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Establishment of strain gradient constitutive relations by homogenization

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ABSTRACT

In this Note, we describe a homogenization methodology with the aim of establishing strain gradient constitutive relations for heterogeneous materials. The presented methodology includes two main steps. The first one is the construction of the average strain-energy density for a well-chosen Representative Volume Element (RVE) by using a homogenization technique. The second one is the transformation of the obtained average strain-energy density to that of the continuum. This transformation permits to ensure that the effective moduli do not depend on the size of an RVE, but only on the intrinsic size of the components. It also ensures that the moduli related to the strain gradient vanish as the contrast between the components disappears. These features were then illustrated by means of a simple example.

RÉSUMÉ

Dans cette Note, nous décrivons une méthodologie d'homogénéisation dans le but d'établir des lois de comportement au gradient de déformation pour les matériaux hétérogènes. La méthodologie présentée comporte deux étapes. La première étape est la construction de la densité moyenne d'énergie de déformation pour un Volume Élémentaire Représentatif (VER) en utilisant une technique d'homogénéisation. La deuxième est de transformer cette densité moyenne obtenue pour un VER en celle valable pour un milieu continu. Cette transformation permet de garantir que les modules effectifs généralisés ne dépendent pas de la taille du VER mais seulement des tailles intrinsèques des constituants. Elle garantit également que les modules du second ordre s'annulent si le contraste entre les propriétés des constituants disparaît. Ces aspects sont illustrés ensuite par un exemple simple.

1. Introduction

In this Note, we develop a homogenization methodology with which strain gradient constitutive relations can be established by means of homogenization over a Representative Volume Element (RVE). This work is mainly motivated by the need of regularized damage models in order to describe size effect or to avoid mesh-dependent results in numerical simulations. In the literature, a wide variety of damage models have been proposed on the basis of continuum damage mechanics [1] by introducing length parameters in constitutive relations. Pijaudier-Cabot and Bazant [2] developed a practical nonlocal model in a continuum damage setting. The development of nonlinear gradient models has taken place predominately in plasticity [3–5]. These gradient theories have afterwards been transferred to damage mechanics [6–8]. Alternative damage gradient models were also developed [9,10]. However, it has to be noticed that in most of these damage models, the length parameters were only adopted for numerical convenience. Their physical meanings in constitutive equations and their microscopic

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origin incite always debates and discussions. In general, the length parameters introduced in these models can't be obtained by conventional homogenization methods.

Numerous authors believe that the homogenization of an RVE by including the gradient terms of the macroscopic field is a natural way to describe the behavior of heterogeneous materials. Drugan [11] and Drugan and Willis [12] developed a non-local effective constitutive equation for a class of linearly elastic composites by formally solving the equilibrium equation. For periodic linearly elastic media, an asymptotic solution technique has been used to obtain the homogenized higher-order gradient material behavior, for which effective moduli up to an arbitrary order may be determined based on the properties and morphology of the phases [13,14]. Multi-scale finite element method was also be used to establish the higher-order macroscopic constitutive tangents [15,16]. This idea was also applied for homogenization of elastic-plastic materials [17] or gradient materials [18]. Apart from these strain gradient laws, another class of strain gradient constitutive laws, namely the Cosserat relationship, can also be obtained by homogenization procedure [19–22].

Even though a number of works have been performed in this topic, some fundamental aspects concerning the uniqueness and the consistence of the higher-order gradient laws issued from homogenization have not been thoroughly studied. For example, the dependence of higher-order effective moduli on the size of the RVE has not been well discussed in the literature. This constitutes the main motivation of the present work.

In the present work, we have established a methodology for the construction of constitutive laws of an elastic heterogeneous material by using the homogenization theory. First, several hypotheses have been adopted in order to adapt the concept of macro-homogeneity in homogenization with higher-order gradients. In addition, we developed a special procedure with the purpose of transforming the constitutive laws for individual RVEs to those for the continuum. This transformation permits to ensure that the effective moduli do not depend on the size of an RVE, but only on the intrinsic size of the components. It also ensures that the moduli related to the strain gradient vanish as the contrast between the components disappears. These features were then illustrated by means of a simple example.

2. Principal hypotheses

The concept of the macro-homogeneity is a fundamental hypothesis in conventional homogenization theory [23]. According to this concept, the stress and strain fields in all points of a body are assumed to admit two different scales of variation. First, they fluctuate in a local microscopic scale. Second, the volume averages of stress and strain fields are nearly uniform in the vicinity of an RVE, and significantly vary only in a macroscopic scale much larger than the dimension of the RVE.

However, this fundamental hypothesis is no longer valid in numerous cases, especially when the macroscopic stress or strain fields can no longer be regarded as uniform in an RVE. In these cases, their gradients cannot be neglected in homogenization procedure.

In order to adapt the macro-homogeneity concept to the cases when higher-order gradients cannot be neglected, we admit the following hypotheses:

1. An RVE is no longer considered as an infinitesimal volume in macroscopic scale. A macroscopic solid Ω is constituted by a finite number of RVEs. Therefore we assume that

$$\Omega = \bigcup \Omega^{(m)}, \qquad \bigcap \Omega^{(m)} = \emptyset, \quad m = 1, M \tag{1}$$

where $\Omega^{(m)}$ is the m-th RVE and M is the total number of the RVEs in Ω.

2. Higher-order strain gradients have no influence on constitutive laws if the material is perfectly homogeneous. If an RVE is constituted of several linearly elastic phases, we can assume that each phase is perfectly homogeneous. As a consequence, for each phase we can write:

$$\begin{cases} \sigma_{ij,j}^{(m)}(\mathbf{y}) + f_i^{(m)}(\mathbf{y}) = 0, \\ \sigma_{ij}^{(m)}(\mathbf{y}) = C_{ijpq}^{(m)}(\mathbf{y}) u_{p,q}^{(m)}(\mathbf{y}), \end{cases} \quad \mathbf{y} \in \Omega^{(m)} \tag{2}$$

where $\sigma^{(m)}(\mathbf{y})$, $\mathbf{u}^{(m)}(\mathbf{y})$, $\mathbf{f}^{(m)}(\mathbf{y})$ are the fluctuating microscopic fields within $\Omega^{(m)}$, respectively the Cauchy stress tensor, the displacement vector and the body force vector; $\mathbf{C}^{(m)}(\mathbf{y})$ is the stiffness tensor, constant in each phase; $\mathbf{y}$ is the local coordinate position associated with the RVE and originated at its geometrical center. In the following, we will distinguish the local coordinate $\mathbf{y}$ from the global one $\mathbf{x}$, associated to the solid Ω. Eq. (2) is the starting point for the construction of high order constitutive laws as suggested by numerous authors [11–22].

3. We assume that there exists a macroscopic displacement field $\mathbf{u}$ issued from smoothing the oscillating microscopic displacement field. The equivalence of these two fields is guaranteed by the equality of their average gradients over an RVE until order n, namely

$$\bar{u}_i = \bar{u}_i^{(m)}, \qquad \overline{\frac{\partial u_i}{\partial x_{j_1}}} = \overline{\frac{\partial u_i^{(m)}}{\partial x_{j_1}}} \cdots \overline{\frac{\partial^n u_i}{\partial x_{j_1} \cdots \partial x_{j_n}}} = \overline{\frac{\partial^n u_i^{(m)}}{\partial x_{j_1} \cdots \partial x_{j_n}}} \tag{3}$$

where the over-bars signify "averaging over $\Omega^{(m)}$". It is to notice that only the two first equalities in (3) are needed in conventional homogenization method.

4. The macroscopic displacement field in $\Omega^{(m)}$ can be represented in terms of its gradients at the geometrical center $\mathbf{x}_c$ by expanding it into a Taylor's series [6,24], namely,

$$u_i(\mathbf{y}) = \frac{\partial u_i(\mathbf{x}_c)}{\partial x_j} y_j + \frac{1}{2}\frac{\partial^2 u_i(\mathbf{x}_c)}{\partial x_j \partial x_k} y_j y_k + \frac{1}{6}\frac{\partial^3 u_i(\mathbf{x}_c)}{\partial x_j \partial x_k \partial x_l} y_j y_k y_l + \cdots, \quad \mathbf{y} \in \Omega^{(m)} \tag{4}$$

where $\frac{\partial u_i(\mathbf{x}_c)}{\partial x_j}$, $\frac{\partial^2 u_i(\mathbf{x}_c)}{\partial x_j \partial x_k}$ and $\frac{\partial^3 u_i(\mathbf{x}_c)}{\partial x_j \partial x_k \partial x_l}$ are the derivatives of the macroscopic displacement at the geometrical center of $\Omega^{(m)}$. The rigid body movement is omitted from (4). According to (4), we can calculate the averages of the derivatives of the macroscopic displacement over $\Omega^{(m)}$, namely:

$$\begin{aligned}
\bar{u}_{i,j} &= \frac{1}{V^{(m)}} \int_{\Omega^{(m)}} u_{i,j}\,\mathrm{d}V = \frac{\partial u_i(\mathbf{x}_c)}{\partial x_j} + \frac{\partial^2 u_i(\mathbf{x}_c)}{\partial x_j \partial x_k} \bar{I}_k^{(m)} + \frac{1}{2}\frac{\partial^3 u_i(\mathbf{x}_c)}{\partial x_j \partial x_k \partial x_l} \bar{I}_{kl}^{(m)} + \cdots \\
\bar{u}_{i,jk} &= \frac{1}{V^{(m)}} \int_{\Omega^{(m)}} u_{i,jk}\,\mathrm{d}V = \frac{\partial^2 u_i(\mathbf{x}_c)}{\partial x_j \partial x_k} + \frac{\partial^3 u_i(\mathbf{x}_c)}{\partial x_j \partial x_k \partial x_l} \bar{I}_l^{(m)} + \cdots \\
\bar{u}_{i,jkl} &= \frac{1}{V^{(m)}} \int_{\Omega^{(m)}} u_{i,jkl}\,\mathrm{d}V = \frac{\partial^3 u_i(\mathbf{x}_c)}{\partial x_j \partial x_k \partial x_l} + \cdots
\end{aligned} \tag{5}$$

where $V^{(m)}$ is the volume of $\Omega^{(m)}$ and

$$\bar{I}_k^{(m)} = \frac{1}{V^{(m)}} \int_{\Omega^{(m)}} y_k\,\mathrm{d}V = 0, \qquad \bar{I}_{kl}^{(m)} = \frac{1}{V^{(m)}} \int_{\Omega^{(m)}} y_k y_l\,\mathrm{d}V \tag{6}$$

Consequently, by taking (3), (5) and (6) into account, the Taylor expansion (4) can also be written as:

$$u_i = \bar{u}_{i,j}^{(m)} y_j + \frac{1}{2}\bar{u}_{i,jk}^{(m)} y_j y_k + \frac{1}{2}\bar{u}_{i,jkl}^{(m)} \left(\frac{1}{3} y_k y_l - \bar{I}_{kl}^{(m)}\right) y_j + \cdots, \quad \mathbf{y} \in \Omega^{(m)} \tag{7}$$

Thus we have a link between the macroscopic field and the average gradients of the microscopic field. It is evident that this link can also be established for stress field. In the resolution of local homogenization problems, the average gradients are often taken as remote loads. In conventional homogenization methods, the first term in the expansion is sufficient for this purpose. More terms are needed when higher-order gradients cannot be neglected.

3. Calculation of the average second gradient

In an RVE, the microscopic displacement and its gradients may be discontinuous. As a consequence, their derivatives will present singularities. For example, in the case of a matrix containing inclusions, the strain field is discontinuous across the interfaces, and therefore, the second gradient $u_{i,jk}^{(m)}$ will present singularities which have to be included in the calculation of $\bar{u}_{i,jk}^{(m)}$. It is evident that this is not necessary when the average displacement and its gradients are imposed as boundary conditions. Hereafter, we only consider the calculation of $\bar{u}_{i,jk}^{(m)}$ in the cases when the stress boundary conditions are prescribed.

In order to avoid the manipulation of singularities, we adopt the definition made in [25], according to which the average second gradient of displacement over an RVE can be written as follows

$$\bar{u}_{i,jk}^{(m)} = \frac{1}{2V^{(m)}} \int_{\partial\Omega^{(m)}} \left(u_{i,j}^{(m)} n_k + u_{i,k}^{(m)} n_j\right) \mathrm{d}S \tag{8}$$

where n_j is the outward unit vector of $\partial\Omega^{(m)}$. We can show that for a matrix containing randomly distributed inclusions, Eq. (8) can be simplified as follows:

$$\bar{u}_{i,jk}^{(m)} = \frac{1}{V^{(m)}} \int_{\Omega^{(m)}\setminus\Gamma} u_{i,jk}^{(m)}\,\mathrm{d}V \tag{9}$$

where $\Omega^{(m)}\setminus\Gamma$ denotes $\Omega^{(m)}$ excluding all the interfaces Γ. In order to demonstrate this equation, let us consider a bi-phase RVE occupying a convex domain. Let c be the probability for an arbitrary point belonging to inclusions, i.e., $\mathbf{y} \in \Omega^{(1)}$, then $1 - c$ is the probability of a point belonging to the matrix, i.e., $\mathbf{y} \in \Omega^{(2)}$, where $\Omega^{(m)} = \Omega^{(1)} \cup \Omega^{(2)}$. It follows that $c = V^{(1)}/V^{(m)}$ and $1 - c = V^{(2)}/V^{(m)}$, where $V^{(1)}$ and $V^{(2)}$ are respectively the volumes of $\Omega^{(1)}$ and $\Omega^{(2)}$. Let c_{rs} be the covariance function that, for two sufficiently distant points in $\Omega^{(m)}$, gives the probability to find simultaneously the phase r at point 1 and the phase s at point 2. In the present case, we have $c_{11} = c^2, c_{22} = (1 - c)^2$ and $c_{12} = c_{21} = c(1 - c)$.

We evaluate now $\bar{u}^{(m)}_{1,11}$ under stress boundary condition $\sigma_{ij} = \bar{\sigma}_{ij} + \bar{\sigma}_{ij,k} y_k$ on $\partial\Omega^{(m)}$. It is clear that the stress traction on $\partial\Omega^{(m)}$ must be statically admissible, i.e. $\int_{\partial\Omega^{(m)}} \sigma_{ij} n_j \, \mathrm{d}S + \int_{\Omega^{(m)}} f_i \, \mathrm{d}V = 0$ where f_i is the body force. The derivative $u_{1,1}$ on $\partial\Omega^{(m)}$ is therefore $H_{11ij}(\bar{\sigma}_{ij} + \bar{\sigma}_{ij,k} y_k)$ with $\mathbf{H}(\mathbf{y})$ being the compliance tensor of the material, $\mathbf{H}(\mathbf{y}) = \mathbf{H}^{(1)}$ for inclusions and $\mathbf{H}(\mathbf{y}) = \mathbf{H}^{(2)}$ for matrix. For more convenience, $\partial\Omega^{(m)}$ can be divided into two parts according to the direction of n_1, i.e. $\partial\Omega^{(m)} = \partial\Omega^{(m)}_+ \cup \partial\Omega^{(m)}_-$, where $\partial\Omega^{(m)}_+$ and $\partial\Omega^{(m)}_-$ are respectively the boundaries with positive and negative values of n_1. From (8) and by omitting the parts of $\partial\Omega^{(m)}$ with $n_1 = 0$ and vertexes, we can write:

$$\bar{u}^{(m)}_{1,11} = \frac{1}{V^{(m)}} \left(\int_{\partial\Omega^{(m)}_+} H_{11ij}(\bar{\sigma}_{ij} + \bar{\sigma}_{ij,1} y_1) n_1 \, \mathrm{d}S + \int_{\partial\Omega^{(m)}_-} H_{11ij}(\bar{\sigma}_{ij} + \bar{\sigma}_{ij,1} y_1) n_1 \, \mathrm{d}S \right)$$

$$= \frac{1}{V^{(m)}} \sum_{\substack{r=1,2 \\ s=1,2}} c_{rs} \left(\int_{\partial\Omega^{(m)}_+} H^{(r)}_{11ij}(\bar{\sigma}_{ij} + \bar{\sigma}_{ij,1} y_1) \, \mathrm{d}y_2 \, \mathrm{d}y_3 - \int_{\partial\Omega^{(m)}_-} H^{(s)}_{11ij}(\bar{\sigma}_{ij} + \bar{\sigma}_{ij,1} y_1) \, \mathrm{d}y_2 \, \mathrm{d}y_3 \right) \tag{10}$$

After some simple algebra, we can obtain:

$$\bar{u}^{(m)}_{1,11} = \big(cH^{(1)}_{11ij} + (1-c)H^{(2)}_{11ij}\big)\bar{\sigma}_{ij,1} \tag{11}$$

It is clear that $H^{(1)}_{11ij}\bar{\sigma}_{ij,1} = \bar{u}^{(1)}_{1,11}$ and $H^{(2)}_{11ij}\bar{\sigma}_{ij,1} = \bar{u}^{(2)}_{1,11}$ are respectively the average strain gradient in $\Omega^{(1)}$ and $\Omega^{(2)}$. Consequently:

$$\bar{u}^{(m)}_{1,11} = \frac{V^{(1)}}{V^{(m)}} \bar{u}^{(1)}_{1,11} + \frac{V^{(2)}}{V^{(m)}} \bar{u}^{(2)}_{1,11} = \frac{1}{V^{(m)}} \int_{\Omega^{(1)}} u^{(m)}_{1,11} \, \mathrm{d}V + \frac{1}{V^{(m)}} \int_{\Omega^{(2)}} u^{(m)}_{1,11} \, \mathrm{d}V = \frac{1}{V^{(m)}} \int_{\Omega^{(m)} \setminus \Gamma} u^{(m)}_{1,11} \, \mathrm{d}V \tag{12}$$

Other components of $\bar{u}^{(m)}_{i,jk}$ can similarly be evaluated. Thus Eq. (9) is demonstrated.

For periodic RVEs, this demonstration is not appropriate as the different phases are not randomly distributed in $\Omega^{(m)}$. In this case, Eq. (9) can still be used if $\bar{u}^{(m)}_{i,jk}$ is regarded as an average value of $\bar{u}^{(m)}_{i,jk}$ calculated with all possible periodic RVEs of the same volume.

4. Creation of strain gradient constitutive relations by homogenization

Under the hypotheses adopted in Section 2, we develop a homogenization methodology including two main steps. The first one is the resolution of the local problem (2) for an RVE subjected to gradient loads on its boundary. Due to introduction of strain gradient, the size of the RVE enters into the constitutive law. Therefore, the homogenization analysis in the first step only provides the constitutive relations for the considered RVE. A special procedure must be developed to transform the obtained constitutive relations to those for the continuum. This is the task of the second step.

Step 1: Homogenization. Consider an RVE $\Omega^{(m)}$ loaded with known traction t_i on its exterior boundary $\partial\Omega^{(m)}$. Let δu_i be a virtual kinematically admissible displacement field, as defined in (7) but truncated after the second term. The virtual work of the traction t_i on the virtual displacement δu_i is

$$\delta W^{(m)}_u = \int_{\partial\Omega^{(m)}} t_i \delta u_i \, \mathrm{d}S = \delta\bar{u}^{(m)}_{i,j} \int_{\partial\Omega^{(m)}} t_i y_j \, \mathrm{d}S + \frac{1}{2} \delta\bar{u}^{(m)}_{i,jk} \int_{\partial\Omega^{(m)}} t_i y_j y_k \, \mathrm{d}S \tag{13}$$

Let's define

$$\bar{\sigma}^{(m)}_{ij} = \frac{1}{V^{(m)}} \int_{\partial\Omega^{(m)}} t_i y_j \, \mathrm{d}S$$

$${}^1\bar{\sigma}^{(m)}_{ijk} = \frac{1}{2V^{(m)}} \int_{\partial\Omega^{(m)}} t_i y_j y_k \, \mathrm{d}S \tag{14}$$

By using the boundary condition $t_i = \sigma^{(m)}_{ij} n_j$ and the equilibrium equation $\sigma^{(m)}_{ij,j} = 0$, we obtain:

$$\bar{\sigma}^{(m)}_{ij} = \frac{1}{V^{(m)}} \int_{\Omega^{(m)}} \sigma^{(m)}_{ij} \, \mathrm{d}V$$

$${}^1\bar{\sigma}^{(m)}_{ijk} = \frac{1}{2V^{(m)}} \int_{\Omega^{(m)}} \big(\sigma^{(m)}_{ij} y_k + \sigma^{(m)}_{ik} y_j\big) \, \mathrm{d}V \tag{15}$$

Thus we can see that $\bar{\sigma}_{ij}^{(m)}, {}^1\bar{\sigma}_{ijk}^{(m)}$ are respectively the average stress and double stress tensors over $\Omega^{(m)}$. Using these definitions, Eq. (13) becomes

$$\frac{1}{V^{(m)}} \int\limits_{\partial\Omega^{(m)}} t_i \delta u_i \,\mathrm{d}S = \delta\bar{u}_{i,j}^{(m)} \bar{\sigma}_{ij}^{(m)} + \delta\bar{u}_{i,jk}^{(m)} {}^1\bar{\sigma}_{ijk}^{(m)} \tag{16}$$

The right side of (16) can be regarded as the variation of the average strain energy density $U^{(m)}$ in the RVE defined as follows:

$$\bar{\sigma}_{ij}^{(m)} = \frac{\partial U^{(m)}}{\partial \bar{u}_{i,j}^{(m)}}, \qquad {}^1\bar{\sigma}_{ijk}^{(m)} = \frac{\partial U^{(m)}}{\partial \bar{u}_{i,jk}^{(m)}} \tag{17}$$

Therefore (16) can just read as the virtual work principle applied on $\Omega^{(m)}$:

$$\delta W_u^{(m)} / V^{(m)} = \delta U^{(m)} \tag{18}$$

Eq. (18) is the energy-averaging theorem, known in the literature as the Hill–Mandel condition or macro-homogeneity condition [23,26,27].

The constitutive equations for the RVE can be obtained by solving the local problem (2) under boundary conditions which can be given by the macroscopic displacement or stress fields. The macroscopic constitutive relations are evaluated from (17):

$$\begin{aligned} \bar{\sigma}_{ij}^{(m)} &= \bar{\sigma}_{ij}^{(m)}\big(\bar{u}_{i,j}^{(m)}, \bar{u}_{i,jk}^{(m)}\big) \\ {}^1\bar{\sigma}_{ijk}^{(m)} &= {}^1\bar{\sigma}_{ijk}^{(m)}\big(\bar{u}_{i,j}^{(m)}, \bar{u}_{i,jk}^{(m)}\big) \end{aligned} \tag{19}$$

It is important to point out that Eqs. (19) are obtained from homogenization of a single RVE. Therefore, they are valid only for individual RVEs. In the following, we will rewrite them for a linearly elastic continuum.

Step 2: Transformation. According to Mindlin [28], a strain energy function for a homogeneous and isotropic continuum can be written, using the notation of the present paper, as follows:

$$U = \frac{1}{2}(C_{ijpq} u_{i,j} u_{p,q} + D_{ijkpqr} u_{i,jk} u_{p,qr}) \tag{20}$$

where $u_{i,j}, u_{i,jk}$ are the derivatives of the macroscopic displacement; **C** and **D** are the stiffness tensors for strains and strain gradients. This form of strain energy function can also be found by using the above-mentioned homogenization technique. In fact, for an RVE suitably chosen, we can write the average strain energy density as follows:

$$U^{(m)} = \frac{1}{2}\big(\bar{C}_{ijpq}^{(m)} \bar{u}_{i,j}^{(m)} \bar{u}_{p,q}^{(m)} + \bar{D}_{ijkpqr}^{(m)} \bar{u}_{i,jk}^{(m)} \bar{u}_{p,qr}^{(m)}\big) \tag{21}$$

where $\bar{C}_{ijpq}^{(m)}$, $\bar{D}_{ijkpqr}^{(m)}$ are the average stiffness tensors of the m-th RVE issued from a homogenization procedure.

It is to notice that the form (21) can't be obtained with arbitrary RVEs. The microstructure in a general 3D RVE has to possess at least three orthogonal planes of symmetry with respect to the local coordinate system, at least in a statistical sense. This condition is satisfied for macroscopically isotropic or orthotropic materials with well-chosen RVEs, and also, more generally, for centro-symmetric cells.

The total strain energy in a macroscopic volume Ω is, according to the hypothesis (1) and Eq. (21):

$$\int\limits_{\Omega} U \,\mathrm{d}V = \sum_{m=1}^{M} V^{(m)} \frac{1}{2}\big(\bar{C}_{ijpq}^{(m)} \bar{u}_{i,j}^{(m)} \bar{u}_{p,q}^{(m)} + \bar{D}_{ijkpqr}^{(m)} \bar{u}_{i,jk}^{(m)} \bar{u}_{p,qr}^{(m)}\big) \tag{22}$$

where U is the strain-energy density in Ω. As we pointed above, in general, $U \neq U^{(m)}$ as the later depends on the RVE's volume. Our objective is to transcribe the summation in (22) into an integral expression in order to extract a true strain energy density. To this end, we first consider the integral

$$\int\limits_{\Omega} C_{ijpq} u_{i,j} u_{p,q} \,\mathrm{d}V = \sum_{m=1}^{M} \int\limits_{\bar{\Omega}^{(m)}} C_{ijpq} u_{i,j} u_{p,q} \,\mathrm{d}V \tag{23}$$

where **u** is the macroscopic displacement vector; $\bar{\Omega}^{(m)}$ represents the homogenized RVE, i.e., $\bar{\Omega}^{(m)}$ is a mono-connected domain covering $\Omega^{(m)}$; **C** is the macroscopic stiffness tensor. We assume that it varies very slowly in the scale of an RVE such that $\mathbf{C}(\mathbf{x}) = \bar{\mathbf{C}}^{(m)}$, $\mathbf{x} \in \bar{\Omega}^{(m)}$. In fact, $\mathbf{C}$ is a constant tensor if Ω is constituted of statistically identical RVEs. Thus we can write:

$$\int_{\bar{\Omega}^{(m)}} C_{ijpq}\,\mathrm{d}V = V^{(m)}\bar{C}^{(m)}_{ijpq}, \qquad \int_{\bar{\Omega}^{(m)}} C_{ijpq}\,y_k\,\mathrm{d}V = 0, \qquad \int_{\bar{\Omega}^{(m)}} C_{ijpq}\,y_k y_r\,\mathrm{d}V = \bar{C}^{(m)}_{ijpq}\int_{\bar{\Omega}^{(m)}} y_k y_r\,\mathrm{d}V \tag{24}$$

By truncating (7) after its second term then substituting it into the right side of (23) and by taking (24) into account, we obtain straightforwardly:

$$\sum_{m=1}^{M} V^{(m)}\big(\bar{C}^{(m)}_{ijpq}\bar{u}^{(m)}_{i,j}\bar{u}^{(m)}_{p,q}\big) = \int_{\Omega} C_{ijpq}u_{i,j}u_{p,q}\,\mathrm{d}V - \sum_{m=1}^{M} V^{(m)}\bar{C}^{(m)}_{ijpq}\bar{I}^{(m)}_{kr}\bar{u}^{(m)}_{i,jk}\bar{u}^{(m)}_{p,qr} \tag{25}$$

with

$$\bar{I}^{(m)}_{ij} = \frac{1}{V^{(m)}}\int_{\bar{\Omega}^{(m)}} y_i y_j\,\mathrm{d}V \tag{26}$$

By introducing (25) into (22) we obtain:

$$\int_{\Omega} U\,\mathrm{d}V = \frac{1}{2}\int_{\Omega} u_{i,j}C_{ijpq}u_{p,q}\,\mathrm{d}V + \sum_{m=1}^{M}\frac{V^{(m)}}{2}\big(\bar{D}^{(m)}_{ijkpqr} - \bar{C}^{(m)}_{ijpq}\bar{I}^{(m)}_{kr}\big)\bar{u}^{(m)}_{i,jk}\bar{u}^{(m)}_{p,qr} \tag{27}$$

If the Taylor expansion (7) is truncated after the second term, we have $\bar{u}^{(m)}_{i,jk} = u_{i,jk}$ in $\Omega^{(m)}$. By definition, $u_{i,jk}$ is a slowly varying field in the scale of $\Omega^{(m)}$. Let $\tilde{\mathbf{D}}$ and $\mathbf{I}$ be respectively the macroscopic stiffness tensor and the macroscopic inertia moment tensor. Similarly, we assume that they vary very slowly in the scale of $\Omega^{(m)}$ such that $\tilde{\mathbf{D}}(\mathbf{x}) = \bar{\mathbf{D}}^{(m)}$, $\mathbf{I}(\mathbf{x}) = \bar{\mathbf{I}}^{(m)}$, $\mathbf{x} \in \bar{\Omega}^{(m)}$. It follows that

$$\begin{aligned} V^{(m)}\big(\bar{D}^{(m)}_{ijkpqr} - \bar{C}^{(m)}_{ijpq}\bar{I}^{(m)}_{kr}\big)\bar{u}^{(m)}_{i,jk}\bar{u}^{(m)}_{p,qr} &= \int_{\bar{\Omega}^{(m)}} \big(\bar{D}^{(m)}_{ijkpqr} - \bar{C}^{(m)}_{ijpq}\bar{I}^{(m)}_{kr}\big)\bar{u}^{(m)}_{i,jk}\bar{u}^{(m)}_{p,qrs}\,\mathrm{d}V \\ &= \int_{\bar{\Omega}^{(m)}} (\tilde{D}_{ijkpqr} - C_{ijpq}I_{kr})u_{i,jk}u_{p,qrs}\,\mathrm{d}V \end{aligned} \tag{28}$$

Finally, combining (27) and (28) gives:

$$\int_{\Omega} U\,\mathrm{d}V = \frac{1}{2}\int_{\Omega} (C_{ijpq}u_{i,j}u_{p,q} + D_{ijkpqr}u_{i,jk}u_{p,qr})\,\mathrm{d}V \tag{29}$$

with

$$\begin{aligned} C_{ijpq} &= C^{(m)}_{ijpq} \\ D_{ijkpqr} &= \tilde{D}_{ijkpqr} - C_{ijpq}I_{kr} = \bar{D}^{(m)}_{ijkpqr} - C^{(m)}_{ijpq}I^{(m)}_{kr} \end{aligned} \tag{30}$$

From (29), we extract the strain energy density for macroscopic continuum:

$$U = \frac{1}{2}C_{ijpq}u_{i,j}u_{p,q} + D_{ijkpqr}u_{i,jk}u_{p,qr} \tag{31}$$

Then the constitutive relations in the homogenized continuum are:

$$\begin{aligned} \sigma_{ij} &= \frac{\partial U}{\partial u_{i,j}} = C_{ijpq}u_{p,q} \\ {}^{1}\sigma_{ijk} &= \frac{\partial U}{\partial u_{i,jk}} = D_{ijkpqr}u_{p,qr} \end{aligned} \tag{32}$$

This transformation procedure can be repeated if higher-order gradients are included in the constitutive laws. Eqs. (31) and (32) are of similar form compared with many constitutive laws proposed in the literature. However, the relationships in (31) and (32) are issued from a homogenization consideration, therefore benefit from physical clarity of the method.

As demonstrated above, the gradient constitutive laws involve geometrical parameters of RVEs. However, the gradient constitutive behavior is a material property: Apart from the solution accuracy related to the stochastic aspect of heterogeneities, the size of the RVE should not change the fundamental result of the constitutive behavior. Once the RVEs chosen represent properly the microstructure of the material, adopting different RVEs must provide basically the same constitutive relations. This size-independent feature of the constitutive laws will be checked by the following example.

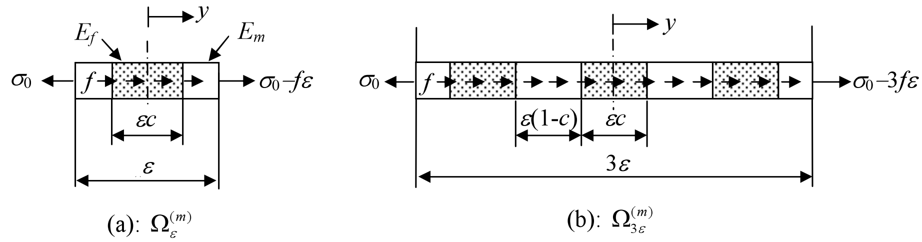

Fig. 1. Two different RVEs "matrix-fibre-matrix".

5. A simple example: one-dimensional composite

Hereafter we will apply the developed homogenization methodology to solve a simple local problem in establishing the strain gradient constitutive relations. The selected example is voluntarily simple with which closed solutions can be obtained. Consider a randomly layered bi-phase bar under uniaxial traction. Let ε_m and ε_f be respectively the average sizes of the matrix and the fibers, thus the average size of a basic cell is $\varepsilon = \varepsilon_m + \varepsilon_f$. Let's also define $c = \varepsilon_f/\varepsilon$ and $1 - c = \varepsilon_m/\varepsilon$ which are respectively the volume ratios of the fibres and the matrix. The Young moduli are denoted by E_f for the fibre phase and E_m for the matrix phase. Beside the external axial tractions at its two extremities, we assume that the bar is also subjected to body forces f, assumed uniform in the composite. For simplicity, the composite bar is considered as an arbitrary combination of two classes of the basic cells: one with the sequence "matrix-fibre-matrix" and another with the sequence "fibre-matrix-fibre".

Let us first consider the RVEs with the sequence "matrix-fibre-matrix". In the following, we will establish the macroscopic constitutive relation for the composite by choosing two different RVEs. The first RVE, named $\Omega_\varepsilon^{(m)}$, is the basic cell and the second, named $\Omega_{3\varepsilon}^{(m)}$, is composed of 3 basic cells, see Fig. 1. The local elasticity problems corresponding to the homogenization on these RVEs are written as follows:

$$\text{Pb1:}\quad \begin{array}{l} \begin{cases} \sigma'^{(m)} + f = 0 \\ \sigma^{(m)} = Eu'^{(m)} \end{cases} \quad \text{for } y \in \Omega_\varepsilon^{(m)} \\ \begin{cases} \sigma^{(m)} = \sigma_0 & \text{at } y = -\varepsilon/2 \\ \sigma^{(m)} = \sigma_0 - f\varepsilon & \text{at } y = \varepsilon/2 \end{cases} \\ u^{(m)}, \sigma^{(m)} \text{ continuous at } y = \pm\varepsilon c/2 \end{array} \tag{33}$$

$$\text{Pb2:}\quad \begin{array}{l} \begin{cases} \sigma'^{(m)} + f = 0 \\ \sigma^{(m)} = Eu'^{(m)} \end{cases} \quad \text{for } y \in \Omega_{3\varepsilon}^{(m)} \\ \begin{cases} \sigma^{(m)} = \sigma_0 & \text{at } y = -3\varepsilon/2 \\ \sigma^{(m)} = \sigma_0 - 3f\varepsilon & \text{at } y = 3\varepsilon/2 \end{cases} \\ u^{(m)}, \sigma^{(m)} \text{ continuous at } y = \pm\varepsilon c/2;\ \pm\varepsilon(1 \pm c)/2 \end{array} \tag{34}$$

For the RVE $\Omega_\varepsilon^{(m)}$, the exact solution of the local problem (33) can be written in closed form. Accounting for the boundary conditions and stress continuity conditions across the interfaces, integration of the equilibrium equation gives:

$$\sigma^{(m)}(y) = -fy + \sigma_0 - f\varepsilon/2 \tag{35}$$

This solution can also be expressed in terms of $\bar{u}'$ and $\bar{u}''$ which are respectively the average macroscopic strain and strain gradient on $\Omega_\varepsilon^{(m)}$. In fact, the equilibrium equation can be written as $u''^{(m)} = -f/E$. Its averaging provides, according to (9),

$$\bar{u}'' = -f/\bar{E} \tag{36}$$

where $\bar{E}$ stands for the homogenized modulus of the composite,

$$\frac{1}{\bar{E}} = \frac{1-c}{E_m} + \frac{c}{E_f} \tag{37}$$

By averaging the strain $u'^{(m)} = \sigma^{(m)}/E^{(m)}$, we have

$$\sigma_0 = \bar{E}\big(\bar{u}' - \bar{u}''\varepsilon/2\big) \tag{38}$$

By substituting (36) and (38) into (35), we obtain:

$$\sigma^{(m)}(y) = \bar{E}\big(\bar{u}' + \bar{u}''y\big) \tag{39}$$

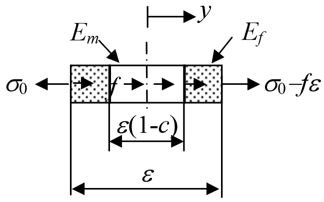

Fig. 2. A fibre-matrix-fibre RVE.

This result allows for the calculation of the average strain energy density on $\Omega_\varepsilon^{(m)}$:

$$U_1^{(m)} = \frac{1}{\varepsilon}\int_{-\frac{\varepsilon}{2}}^{\frac{\varepsilon}{2}} \frac{(\sigma^{(m)})^2}{2E^{(m)}}\,\mathrm{d}y = \frac{1}{2}\bar{E}\big(\bar{u}'\big)^2 + \frac{1}{2}l_1^2\bar{E}\big(\bar{u}''\big)^2 \tag{40}$$

where l_1 is a characteristic length, $l_1^2 = \frac{\bar{E}\varepsilon^2}{12}(\frac{1-c^3}{E_m} + \frac{c^3}{E_f})$.

For the RVE $\Omega_{3\varepsilon}^{(m)}$, the solution of the problem (34) yields the same stress field as in (39). The only difference resides in the calculation of $\bar{u}'$ and $\bar{u}''$, given by $\sigma_0 = \bar{E}(\bar{u}' - 3\bar{u}''\varepsilon/2)$ and $f = -\bar{E}\bar{u}''$. The average strain energy density in $\Omega_{3\varepsilon}^{(m)}$ is therefore:

$$U_3^{(m)} = \frac{1}{3\varepsilon}\int_{-\frac{3\varepsilon}{2}}^{\frac{3\varepsilon}{2}} \frac{(\sigma^{(m)})^2}{2E^{(m)}}\,\mathrm{d}y = \frac{1}{2}\bar{E}\big(\bar{u}'\big)^2 + \frac{1}{2}l_3^2\bar{E}\big(\bar{u}''\big)^2 \tag{41}$$

with $l_3^2 = l_1^2 + \frac{2}{3}\varepsilon^2$.

It is clear that $U_1^{(m)} \neq U_3^{(m)}$ even though $\Omega_\varepsilon^{(m)}$ and $\Omega_{3\varepsilon}^{(m)}$ can both represent the microstructure of the composite. The constitutive laws thus obtained depend on the volume of the RVE if the strain gradient $\bar{u}''$ is taken into account. Moreover, the strain gradient terms still exist in these expressions when $E_m = E_f$, that is in contradiction with the common knowledge. These anomalies can be remedied by using the transformation method described in Section 4.

According to the second equation in (32), we can calculate the effective stiffness for the strain gradient term, namely:

For $\Omega_\varepsilon^{(m)}$:

$$D = \bar{E}l_1^2 - \bar{E}\frac{1}{\varepsilon}\int_{\bar{\Omega}_\varepsilon^{(m)}} y^2\,\mathrm{d}y = \bar{E}^2\varepsilon^2\left(\frac{1-c^3}{12E_m} + \frac{c^3}{12E_f}\right) - \frac{\bar{E}\varepsilon^2}{12} = \frac{\varepsilon_m\varepsilon_f(1+c)\bar{E}^2}{12}\left(\frac{1}{E_m} - \frac{1}{E_f}\right) \tag{42}$$

For $\Omega_{3\varepsilon}^{(m)}$:

$$D = \bar{E}l_3^2 - \frac{\bar{E}}{3\varepsilon}\int_{\bar{\Omega}_{3\varepsilon}^{(m)}} y^2\,\mathrm{d}y = \bar{E}\varepsilon^2\left(\frac{\bar{E}}{E_m}\frac{1-c^3}{12} + \frac{\bar{E}}{E_f}\frac{c^3}{12} + \frac{2}{3}\right) - \frac{3}{4}\bar{E}\varepsilon^2 = \frac{\varepsilon_m\varepsilon_f(1+c)\bar{E}^2}{12}\left(\frac{1}{E_m} - \frac{1}{E_f}\right) \tag{43}$$

By applying this transformation procedure, we do obtain the same constitutive equation from the homogenization of two RVEs of different size. The strain energy density is therefore:

$$U^{(matrix\text{–}fibre\text{–}matrix)} = \frac{\bar{E}}{2}\left[\big(u'\big)^2 + \frac{\varepsilon_m\varepsilon_f(1+c)\bar{E}}{12}\left(\frac{1}{E_m} - \frac{1}{E_f}\right)\big(u''\big)^2\right] \tag{44}$$

With this result, the strain energy density for an RVE with the sequence “fibre-matrix-fibre” (Fig. 2) can easily be obtained just by exchanging c with $(1-c)$ and E_m with E_f in Eq. (44), thus we have:

$$U^{(fibre\text{–}matrix\text{–}fibre)} = \frac{\bar{E}}{2}\left[\big(u'\big)^2 + \frac{\varepsilon_m\varepsilon_f(2-c)\bar{E}}{12}\left(\frac{1}{E_f} - \frac{1}{E_m}\right)\big(u''\big)^2\right] \tag{45}$$

Since the probability of the sequence “matrix-fibre-matrix” is $1-c$ and the probability of the sequence “fibre-matrix-fibre” is c, the average strain energy density of the composite writes:

$$U = (1-c)U^{(matrix\text{–}fibre\text{–}matrix)} + cU^{(fibre\text{–}matrix\text{–}fibre)} = \frac{\bar{E}}{2}\left[\big(u'\big)^2 + \frac{\varepsilon_m\varepsilon_f(1-2c)\bar{E}}{12}\left(\frac{1}{E_m} - \frac{1}{E_f}\right)\big(u''\big)^2\right] \tag{46}$$

From Eq. (46), the following remarks can be made:

1. The strain gradient term in the density of strain energy is directly related to the size, volume ratio and stiffness of each component of the composite, but independent of the RVE's size.
2. The strain gradient term disappears if the difference between E_m and E_f vanishes.
3. When the matrix and the fibres have identical volume ratio ($c = 1/2$), the strain gradient term vanishes.
4. When the components in the bar are randomly distributed, unique constitutive law can be obtained. However, when the composition of the bar is periodic, the homogenization results are not unique. In this case, the strain gradient term depends on the choice of the RVE.
5. The gradient term can be either positive or negative. When the volume of fibers is smaller than that of matrix ($c < 1/2$), this term is positive when the fibre is stronger than the matrix ($E_f > E_m$), and negative in the contrary ($E_f < E_m$).

We recognize that these results are rather new and their correct interpretation requires more detailed analysis.

It is worthy to notice that more complicated 2D or 3D problems can also be studied with the proposed methodology, and similar results can be obtained. However, they are not presented in this Note in order to save space.

6. Concluding remarks

In this paper, we first developed a homogenization procedure in order to establish strain gradient constitutive relations for a heterogeneous material. The main hypotheses adopted in this approach include the consideration of an RVE as a volume with finite size and the inexistence of gradient behavior if the material is perfectly homogeneous. An important feature of the present method is its self-consistency with respect to the selection of the RVE. Once the microstructure of the material is correctly represented in an RVE, the constitutive equations obtained by using the present method are independent of its size. This aspect was illustrated by a simple example in which a one-dimensional periodic composite was homogenized by including strain gradient.

It is clear that the present Note deals with a very open problem which still requires great research efforts on many fundamental and application aspects. One of the research directions may be the development of micromechanics-based high-order constitutive laws with the micro-flaws' size as internal variable. This class of constitutive laws can be used as the base in the establishment of regularized damage models, which allow, on the one hand, a realistic description of the size effect, and on the other hand, mesh-independent finite element simulations.

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