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On two micromechanics theories for determining micro–macro relations in heterogeneous solids

Muneo Hori^a, Sia Nemat-Nasser^{b,*}

^a Earthquake Research Institute, University of Tokyo, 1-1-1 Yayoi Bunkyo, Tokyo 113-0032, Japan

^b Department of AMES, Center of Excellence for Advanced Materials, University of California, 0416, 9500 Gilman Drive, La Jolla, San Diego, CA 92093-0416, USA

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Abstract

The average-field theory and the homogenization theory are briefly reviewed and compared. These theories are often used to determine the effective moduli of heterogeneous materials from their microscopic structure in such a manner that boundary-value problems for the macroscopic response can be formulated. While these two theories are based on different modeling concepts, it is shown that they can yield essentially the same effective moduli and boundary-value problems. A hybrid micromechanics theory is proposed in view of this correspondence. This theory leads to a more accurate computation of the effective moduli, and applies to a broader class of microstructural models. Hence, the resulting macroscopic boundary-value problem gives better estimates of the macroscopic response of the material. In particular, the hybrid theory can account for the effects of the macrostrain gradient on the macrostress in a natural manner. © 1999 Elsevier Science Ltd. All rights reserved.

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1. Introduction

One major objective of micromechanics of heterogeneous materials is to determine the effective overall properties by certain microscopic considerations. The effective properties are then used to evaluate the response of structural elements which consist of heterogeneous materials. Consider two basic approaches for obtaining the overall response of a heterogeneous medium: (1) the *average-field theory* (or the *mean-field theory*) and (2) the *homogenization theory*. Roughly

speaking, these are physics- and mathematics-based theories, respectively. Here, the basic characters of these two theories are interpreted as follows:

Average-field theory. This theory is based on the fact that the effective mechanical properties measured in experiments are relations between the volume average of the strain and stress of microscopically heterogeneous samples. Hence, macrofields are defined as the volume averages of the corresponding microfields, and the effective properties are determined as relations between the averaged microfields.

Homogenization theory. This theory establishes mathematical relations between the microfields and the macrofields, using a multi-scale

* Corresponding author. Tel.: +1-619-534-4772; fax: +1-619-534-2727; e-mail: sia@halebopp.ucsd.edu

perturbation method. The effective properties then naturally emerge as consequences of these relations, without depending on specific physical measurements.

Nemat-Nasser and Hori (1993) presents a concise list of references related to the average-field theory and the homogenization theory; see also Hill (1963), Mura (1987) for the average-field theory. Sanchez-Palencia (1981) and Bakhvalov and Panasenko (1984) present the homogenization theory; see also Nuna and Keller (1984), Walker et al. (1991); see, for instance, Hornung (1996), Kevorkina and Cole (1996) and Terada et al. (1996) for recent works.

Thus, fundamentally, the average-field theory and the homogenization theory deal with the relation between the macrofields and the microfields in different manners. Hence, it seems that the two theories are basically different. Furthermore, their modeling of the microstructure is also different: the homogenization theory usually uses a periodic microstructure as a model, being mainly applied to composite materials with more or less regularly arranged microstructure, whereas the average-field theory often uses simple microstructure models, such as an isolated inclusion in an unbounded body, in order to determine the effective properties.

It is possible to formulate the homogenization theory in a setting which produces the effective properties identical to those obtained through the application of the average-field theory. Furthermore, it is possible to combine the two theories to develop a more general theory which is capable of rigorously predicting the effective properties even when the strain gradients are very large and the average-field theory may no longer apply.

In this paper, we are primarily concerned with establishing a link between the average-field theory and the homogenization theory, clarifying their similarities and differences. A new micromechanics theory is then proposed as a hybrid of these theories. The content of this paper is as follows: First, Section 2 clarifies the problem setting to which the two micromechanics theories are applied; a heterogeneous elastic body with elastic moduli varying in a very small length scale is considered as an example. The formulation of the problem using

the average-field theory and the homogenization theory is then presented in Sections 3 and 4, respectively; similar boundary-value problems are obtained for the two cases even though the underlying assumptions and the method of derivation are different. The resulting boundary-value problems are compared, and a new micromechanics theory is proposed as the hybrid of these two theories in Sections 5 and 6.

Symbolic and index notations are used in this paper; for instance, stress tensor is denoted by either $\boldsymbol{\sigma}$ or σ_{ij} . In the symbolic notation, \cdot and $:$ stand for the first- and second-order contractions, and \otimes for the tensor product. In the index notation, the summation convention is employed.

2. Problem setting

We consider a linearly elastic body, B , which consists of heterogeneous materials; see Fig. 1. Let D and d be the macro- and micro-length scales; D is regarded as the dimension of a sample of the heterogeneous material which is used in experiments, and d is the size of typical micro constituents of this sample. The length scale of B is orders¹ of magnitude greater than that of macro-length scale. We define a relative length scale parameter, ε , as follows:

$$\varepsilon = \frac{d}{D} \ll 1. \quad (1)$$

Let $\mathbf{C}^\varepsilon = \mathbf{C}^\varepsilon(\mathbf{X})$ be the variable elasticity tensor of B , where \mathbf{X} denotes a continuum point in B . Here, superscript ε emphasizes that the variation of this elasticity tensor is measured at the relative scale of ε . Displacement, strain, and stress fields of B are denoted by $\mathbf{u}^\varepsilon = \mathbf{u}^\varepsilon(\mathbf{X})$, $\boldsymbol{\epsilon}^\varepsilon = \boldsymbol{\epsilon}^\varepsilon(\mathbf{X})$, and $\boldsymbol{\sigma}^\varepsilon = \boldsymbol{\sigma}^\varepsilon(\mathbf{X})$, respectively. These fields satisfy

¹ To give an insight to the length scale, consider a case when B is analyzed by the finite element method. In the three dimensional analysis, B is discretized by using $(10^1 \sim 10^3)^3$ elements. Each element corresponds to an RVE. Since D corresponds to the element size, d becomes $\varepsilon(10^{-1} \sim 10^{-3})$ of the size of B . As is seen, a huge computation capacity is required to compute the response of B and each microconstituent simultaneously.

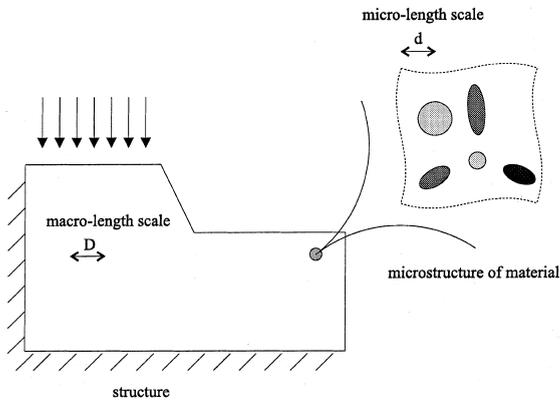


Fig. 1. Boundary value problem for body consisting of material with microstructure.

$$\epsilon^e(\mathbf{X}) = \text{sym}\{\nabla \otimes \mathbf{u}^e(\mathbf{X})\}, \quad (2)$$

$$\nabla \cdot \sigma^e(\mathbf{X}) = 0, \quad (3)$$

$$\sigma^e(\mathbf{X}) = \mathbf{C}^e(\mathbf{X}) : \epsilon^e(\mathbf{X}), \quad (4)$$

where sym stands for the symmetric part, i.e., $\text{sym}\{(\cdot)_{,ij}\} = ((\cdot)_{,ij} + (\cdot)_{,ji})/2$. When B is subjected to, say, surface displacements, $\mathbf{u} = \mathbf{u}^0$ on ∂B , these three sets of the field equations yield the following boundary-value problem for \mathbf{u}^e :

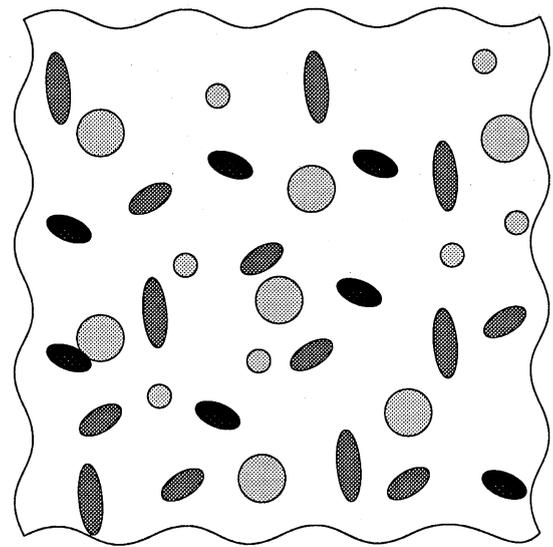
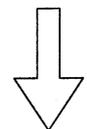
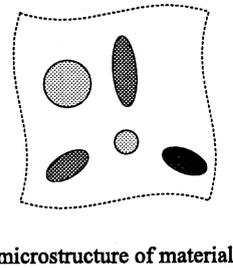
$$\begin{aligned} \nabla \cdot (\mathbf{C}^e(\mathbf{X}) : (\nabla \otimes \mathbf{u}^e(\mathbf{X}))) &= 0 && \text{in } B, \\ \mathbf{u}^e(\mathbf{X}) &= \mathbf{u}^0(\mathbf{X}) && \text{on } \partial B. \end{aligned} \quad (5)$$

The boundary-value problem (5) cannot be solved in its present form, because \mathbf{C}^e changes within a micro-length scale d while the dimensions of B are orders of magnitude greater than d , requiring an unreasonable numerical effort. We consider a micromechanics theory which resolves this difficulty. Since ϵ^e and σ^e vary within the scale of d , such a theory usually introduces strain and stress fields which change within the scale of D . We call the fields varying within the scale of D *macrofields*, and those varying within the scale of d *microfields*.

3. Average-field theory

The average-field theory starts by introducing a *representative volume element*, denoted by V , as

a body which models the microstructure of a given heterogeneous material; see Fig. 2. While various definitions (See Nemat-Nasser and Hori (1993)) are possible, we regard a representative volume element as a model of a sample of the material to be used to determine the corresponding effective properties experimentally. The effective properties are given as relations between the strains and stresses of the sample. These



statistically homogeneous representative volume element

Fig. 2. Representative volume element as model of material with microstructure.

strains and stresses are measured from the sample's surface displacements and tractions, respectively. It is easily shown that these strains and stresses are actually the volume average of the corresponding field variables within the samples. Indeed, applying the averaging theorems² for a compatible strain and a self-equilibrating stress, ϵ and σ , we obtain

$$\langle \epsilon \rangle_V = \frac{1}{V} \int_{\partial V} \text{sym}\{\mathbf{v} \otimes \mathbf{u}\} \, dS, \quad (6)$$

$$\langle \sigma \rangle_V = \frac{1}{V} \int_{\partial V} \mathbf{t} \otimes \mathbf{x} \, dS, \quad (7)$$

where $\langle \cdot \rangle_V$ stands for the volume average taken over V , \mathbf{v} is the outer unit normal on the boundary ∂V , and \mathbf{u} and \mathbf{t} are the surface displacement and traction. These equalities hold for any arbitrary material with any constitutive properties.

3.1. Macrofields of average-field theory

Based on Eqs. (6) and (7), the average-field theory defines macrofield variables as weighted averages of the corresponding microfield variables in the representative volume element. The weight function, denoted by $\phi_V = \phi_V(\mathbf{x})$, satisfies $\int \phi_V \, dV = 1$, and takes on a constant value of $1/V$ within V except for a thin layer near ∂V where it decays smoothly from $1/V$ to 0 on ∂V ; the size of V is of the order of D . The macrodisplacement, macrostrain, and macrostress fields are thus expressed in terms of ϕ_V and the corresponding microfields, as

$$\begin{pmatrix} \mathbf{U}^e(\mathbf{X}) \\ \mathbf{E}^e(\mathbf{X}) \\ \boldsymbol{\Sigma}^e(\mathbf{X}) \end{pmatrix} = \int_B \phi_V(\mathbf{X} - \mathbf{Y}) \begin{pmatrix} \mathbf{u}^e(\mathbf{Y}) \\ \boldsymbol{\epsilon}^e(\mathbf{Y}) \\ \boldsymbol{\sigma}^e(\mathbf{Y}) \end{pmatrix} \, dV_Y. \quad (8)$$

² The averaging theories are easily proved by applying the integral by part and the Gauss theorem in computing the volume average of field variables.

The averaging with the weight ϕ_V cancels possible high oscillations of the field variables which may occur within a micro-length scale.

Since ϕ_V in Eq. (8) is defined as a smooth function, it follows from Eqs. (2) and (3) that the macrostrain and macrostress fields satisfy

$$\mathbf{E}^e(\mathbf{X}) = \text{sym}\{\nabla \otimes \mathbf{U}^e(\mathbf{X})\}, \quad (9)$$

$$\nabla \cdot \boldsymbol{\Sigma}^e(\mathbf{X}) = 0. \quad (10)$$

Therefore, if a constitutive relation between \mathbf{E}^e and $\boldsymbol{\Sigma}^e$ is given, a governing equation which determines the variation of \mathbf{U}^e in B can be obtained from Eqs. (9) and (10). For instance, if an effective elasticity tensor of the homogeneous material is found such that

$$\boldsymbol{\Sigma}^e(\mathbf{X}) = \bar{\mathbf{C}} : \mathbf{E}^e(\mathbf{X}), \quad (11)$$

then, the three sets of the field equations for the macrofields, namely, Eqs. (9)–(11), yield the following governing equation for \mathbf{U}^e :

$$\nabla \cdot (\bar{\mathbf{C}} : (\nabla \otimes \mathbf{U}^e(\mathbf{X}))) = 0 \text{ in } B. \quad (12)$$

Hence, a boundary-value problem for \mathbf{U}^e is obtained by assuming $\mathbf{u}^e \approx \mathbf{U}^e$ near ∂B , i.e., $\mathbf{U}^e = \mathbf{u}^0$ on ∂B .

The effective elasticity tensor, $\bar{\mathbf{C}}$, which appears in Eq. (11) relates the volume average of the microstrains to that of the microstresses. For a two-phase composite material, $\bar{\mathbf{C}}$ is expressed in terms of a *strain concentration tensor*, \mathbf{A} , which relates the average strain of the inclusion phase, $\langle \epsilon \rangle_I$, to that of the composite (or, equally, the representative volume element), $\langle \epsilon \rangle_V$, through $\langle \epsilon \rangle_I = \mathbf{A} : \langle \epsilon \rangle_V$, as follows:

$$\bar{\mathbf{C}} = \mathbf{C}^M + f(\mathbf{C}^I - \mathbf{C}^M) : \mathbf{A}. \quad (13)$$

Here, \mathbf{C}^M and \mathbf{C}^I are the elasticity of the matrix and inclusion phases, respectively, and f is the volume fraction of the inclusion phase; see Appendix A. In the average-field theory, the strain concentration tensor is estimated by using various averaging schemes such as the dilute distribution assumption, the self-consistent method, or the Mori–Tanaka method; see Nemat-Nasser and Hori (1993) and Hori and Nemat-Nasser (1993) for the averaging schemes.

3.2. Statistical homogeneity

The heterogeneous material needs to be *statistical homogeneous*³ in order for Eq. (11) to hold at a point inside of the body B , i.e., in order that the (weighted) average strain and stress be related through an effective elasticity tensor which is common to all points within B .

The effective elasticity tensor, $\bar{\mathbf{C}}$, which is defined from the relation between the average stress and the average strain, is also required to give a relation between the average strain energy and the average strain, i.e.,

$$\begin{aligned} \frac{1}{2} \mathbf{E}^e(\mathbf{X}) : \bar{\mathbf{C}} : \mathbf{E}^e(\mathbf{X}) \\ = \int_B \phi_V(\mathbf{X} - \mathbf{Y}) \left(\frac{1}{2} \boldsymbol{\epsilon}^e(\mathbf{Y}) : \mathbf{C}^e(\mathbf{Y}) : \boldsymbol{\epsilon}^e(\mathbf{Y}) \right) dV_Y. \end{aligned} \quad (14)$$

To obtain conditions for Eq. (14) to be valid, we use the averaging theorem for the strain energy,

$$\langle \boldsymbol{\epsilon} : \boldsymbol{\sigma} \rangle_V = \frac{1}{V} \int_{\partial V} \mathbf{t} \cdot \mathbf{u} \, dS, \quad (15)$$

which leads to

$$\begin{aligned} \langle \boldsymbol{\epsilon} : \boldsymbol{\sigma} \rangle_V - \langle \boldsymbol{\epsilon} \rangle_V : \langle \boldsymbol{\sigma} \rangle_V \\ = \frac{1}{V} \int_{\partial V} (\mathbf{u} - \mathbf{x} \cdot \langle \boldsymbol{\epsilon} \rangle) \cdot (\mathbf{t} - \mathbf{v} \cdot \langle \boldsymbol{\sigma} \rangle) \, dS. \end{aligned} \quad (16)$$

It is shown that if V is a subdomain of a material which consists of more or less similar microstructures, the right side of Eq. (16) decays to 0 as the size of V increases. Since the average weighted by ϕ_V is almost the same as the unweighted volume average, we can assume that Eq. (14) holds when a sufficiently large representative volume element is taken from a composite with a statistically homogeneous microstructure.

For the homogeneous strain or stress boundary conditions, $\mathbf{u} = \mathbf{x} \cdot \boldsymbol{\epsilon}^0$ or $\mathbf{t} = \mathbf{v} \cdot \boldsymbol{\sigma}^0$ on ∂V , with constant $\boldsymbol{\epsilon}^0$ or $\boldsymbol{\sigma}^0$, the right side of Eq. (16) van-

ishes even if V is not statistically homogeneous. However, the strain and stress fields within V will not be the same for different boundary conditions. This means that the effective elasticity tensor can vary depending on the displacement or traction boundary data on the boundary ∂V . Indeed, the following exact *universal inequalities*⁴ (Nemat-Nasser and Hori, 1993) hold for strain fields of a common volume average

$$\langle \boldsymbol{\epsilon}^\Sigma : \mathbf{C} : \boldsymbol{\epsilon}^\Sigma \rangle_V \leq \langle \boldsymbol{\epsilon}^G : \mathbf{C} : \boldsymbol{\epsilon}^G \rangle_V \leq \langle \boldsymbol{\epsilon}^E : \mathbf{C} : \boldsymbol{\epsilon}^E \rangle_V, \quad (17)$$

where $\boldsymbol{\epsilon}^E$, $\boldsymbol{\epsilon}^G$, and $\boldsymbol{\epsilon}^\Sigma$ are the strain fields with a common volume average when V is subjected to homogeneous strain boundary conditions, general (possibly mixed) boundary conditions, and homogeneous stress boundary conditions, respectively; see Appendix B for the proof of Eq. (17). Fig. 3 presents a schematic view of the universal inequalities. Therefore, the representative volume element must be such that $\langle \boldsymbol{\epsilon}^E : \mathbf{C} : \boldsymbol{\epsilon}^E \rangle_V - \langle \boldsymbol{\epsilon}^\Sigma : \mathbf{C} : \boldsymbol{\epsilon}^\Sigma \rangle_V$ is negligibly small, in order to uniquely define the effective elasticity tensor.

4. Homogenization theory

The homogenization theory considers the governing equations in Eq. (5) for \mathbf{u}^e , and in order to express the changes in \mathbf{C}^e within a micro-length scale, it replaces this elasticity tensor field \mathbf{C}^e by

$$\mathbf{C}^e(\mathbf{X}) \approx \mathbf{C}(\mathbf{x}), \quad (18)$$

with $\mathbf{x} = \varepsilon^{-1} \mathbf{X}$. Usually,⁵ it is assumed that $\mathbf{C}(\mathbf{x})$ is spatially periodic, and a periodic structure is used as a model of the microstructure; see Fig. 4.

³ In a narrower sense, the statistical homogeneity means that a probability of finding a phase at a point does not depend on the point.

⁴ As shown by Nemat-Nasser and Hori (1993), the universal theorems play a key role in rendering rigorous the classical bounds on the effective moduli, developed by Hashin and Shtrikman (1962); see also Walpole (1969), Willis (1977), Francfort and Murat (1986), Milton and Kohn (1988), and Torquato (1991), and Nemat-Nasser and Hori (1995).

⁵ See, for instance, Oleinik et al. (1992) for the homogenization theory of non-periodic media.

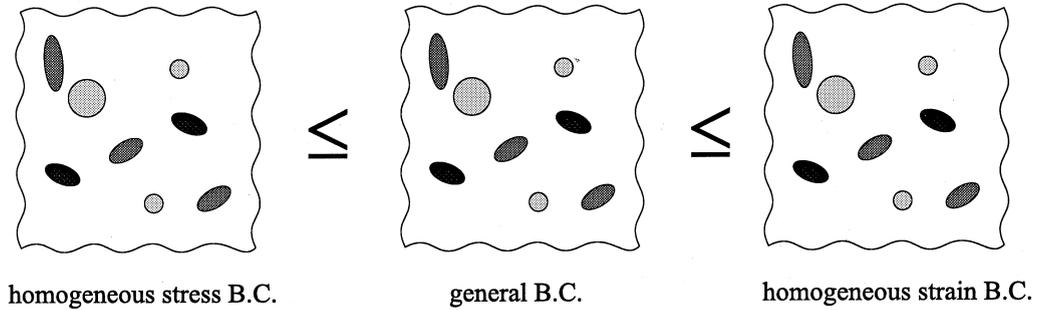


Fig. 3. Universal inequalities.

The dimensions of the unit cell, U , of the periodic structure are of the same order as D .

4.1. Singular perturbation of homogenization theory

For a periodic C , the homogenization theory considers the following multi-scale or singular perturbation representation ⁶ of u^ε :

$$u^\varepsilon(\mathbf{X}) \approx \sum_{n=0} \varepsilon^n u^n(\mathbf{X}, \mathbf{x}), \tag{19}$$

where each u^n has the same periodicity as C with respect to \mathbf{x} . Since ∇ is now replaced by $\nabla_X + \varepsilon^{-1} \nabla_x$, substitution of Eq. (19) into the governing equations of (5) yields

$$\begin{aligned} &\varepsilon^{-2} \{ \nabla_x \cdot (C(\mathbf{x}) : (\nabla_x \otimes u^0(\mathbf{X}, \mathbf{x}))) \} \\ &+ \varepsilon^{-1} \{ \nabla_X \cdot (C(\mathbf{x}) : (\nabla_x \otimes u^0(\mathbf{X}, \mathbf{x}))) \\ &+ \nabla_x \cdot C(\mathbf{x}) : (\nabla_X \otimes u^0(\mathbf{X}, \mathbf{x}) + \nabla_x \otimes u^1(\mathbf{X}, \mathbf{x})) \} \\ &+ \sum_{n=0} \varepsilon^n \{ \nabla_X \cdot (C(\mathbf{x}) : (\nabla_X \otimes u^n(\mathbf{X}, \mathbf{x})) \\ &+ \nabla_x \otimes u^{n+1}(\mathbf{X}, \mathbf{x})) \\ &+ \nabla_x \cdot (C(\mathbf{x}) : (\nabla_X \otimes u^{n+1}(\mathbf{X}, \mathbf{x})) \\ &+ \nabla_x \otimes u^{n+2}(\mathbf{X}, \mathbf{x})) \} = 0. \tag{20} \end{aligned}$$

⁶ In Eq. (19), the perturbation parameter ε is defined as the ratio of the micro-length scale over the macro-length scale. While this parameter is simple, it neglects the change in the magnitude of C ; it is intuitively expected that the perturbation parameter should decrease as, say, the ratio of the maximum and minimum values of each component of C decreases.

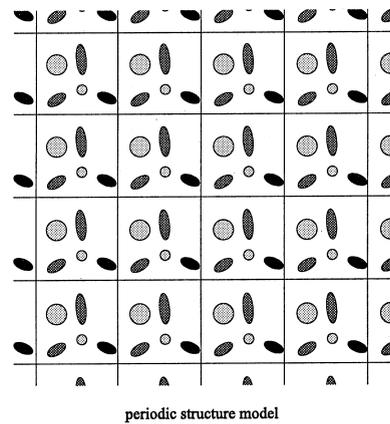
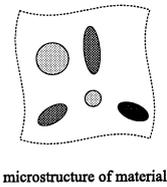


Fig. 4. Periodic structure as model of material with micro-structure.

To solve (20) up to $O(\varepsilon^0)$, the homogenization theory first assumes that u^0 is a function of only \mathbf{X} and that u^1 admits the representation $u^1(\mathbf{X}, \mathbf{x}) = \chi^1(\mathbf{x}) : (\nabla_X \otimes u^0(\mathbf{X}))$, where a third-order tensor χ^1 is periodic with respect to \mathbf{x} . Then, terms of $O(\varepsilon^{-2})$ vanish, and terms of $O(\varepsilon^{-1})$ become

$$\{\nabla_{\mathbf{x}} \cdot (\mathbf{C}(\mathbf{x}) : (\nabla_{\mathbf{x}} \otimes \boldsymbol{\chi}^1(\mathbf{x}) + \mathbf{1}^{(4s)}))\} : (\nabla_{\mathbf{X}} \otimes \mathbf{u}^0(\mathbf{X})),$$

where $\mathbf{1}^{(4s)}$ is the symmetric fourth-order identity tensor. In order for these terms to vanish identically for both \mathbf{X} and \mathbf{x} , $\boldsymbol{\chi}^1$ must satisfy the following governing equation with the periodic boundary conditions

$$\nabla_{\mathbf{x}} \cdot (\mathbf{C}(\mathbf{x}) : (\nabla_{\mathbf{x}} \otimes \boldsymbol{\chi}^1(\mathbf{x}) + \mathbf{1}^{(4s)})) = 0. \quad (21)$$

It is seen that $\boldsymbol{\chi}^1 : (\nabla_{\mathbf{X}} \otimes \mathbf{u}^0)$ is a microscopic displacement field in the presence of the stress field, $\mathbf{C} : (\nabla_{\mathbf{X}} \otimes \mathbf{u}^0)$. Since this stress field does not satisfy equilibrium, oscillating microstrains and associated stresses are produced. In another word, $\boldsymbol{\chi}^1$ corresponds to the microscale response which accommodates the strain field $\text{sym}\{\nabla_{\mathbf{X}} \otimes \mathbf{u}^0\}$ which produces non-equilibrating stresses. Note that $\boldsymbol{\chi}^1$ satisfies the symmetry, $\chi_{ikl}^1 = \chi_{ilk}^1$.

Once $\boldsymbol{\chi}^1$ is determined, terms of $O(\varepsilon^0)$ in Eq. (20) become

$$\begin{aligned} &\nabla_{\mathbf{X}} \cdot \{ \mathbf{C}(\mathbf{x}) : ((\nabla_{\mathbf{x}} \otimes \boldsymbol{\chi}^1(\mathbf{x}) + \mathbf{1}^{(4s)}) : (\nabla_{\mathbf{X}} \otimes \mathbf{u}^0(\mathbf{X}))) \} \\ &+ \nabla_{\mathbf{x}} \cdot \{ \mathbf{C}(\mathbf{x}) : ((\nabla_{\mathbf{x}} \otimes \mathbf{u}^1(\mathbf{X}, \mathbf{x}) \\ &+ \nabla_{\mathbf{x}} \otimes \mathbf{u}^2(\mathbf{X}, \mathbf{x}))) \}. \end{aligned}$$

If the volume average over the unit cell is taken, terms varying with \mathbf{x} drop out, and the governing equation for \mathbf{u}^0 is obtained as

$$\nabla_{\mathbf{X}} \cdot (\overline{\mathbf{C}}^0 : (\nabla_{\mathbf{X}} \otimes \mathbf{u}^0(\mathbf{X}))) = 0 \text{ in } B, \quad (22)$$

with

$$\overline{\mathbf{C}}^0 = \frac{1}{U} \int_U \mathbf{C}(\mathbf{x}) : (\nabla_{\mathbf{x}} \otimes \boldsymbol{\chi}^1(\mathbf{x}) + \mathbf{1}^{(4s)}) \, dV. \quad (23)$$

Therefore, a boundary-value problem for \mathbf{u}^0 is obtained if $\mathbf{u}^0 \approx \mathbf{u}^e$ is assumed and $\mathbf{u}^0 = \mathbf{u}^0$ is prescribed as the boundary conditions on ∂B .

4.2. Macrofields of homogenization theory

Since the leading term of the perturbation expansion, \mathbf{u}^0 , is a function of only \mathbf{X} , it corresponds to the macrodisplacement in the average-field theory. The next term, $\varepsilon \mathbf{u}^1$, contributes little, as it is of

the order of $O(\varepsilon^1)$. Indeed, the volume average of $\mathbf{u}^1 = \boldsymbol{\chi}^1 : (\nabla_{\mathbf{X}} \otimes \mathbf{u}^0)$ taken over U vanishes since $\boldsymbol{\chi}^1$ is periodic.

A singular perturbation expansion similar to Eq. (19) is applicable to the strain and stress fields, i.e., $\{\boldsymbol{\varepsilon}^e, \boldsymbol{\sigma}^e\} = \sum_{n=0} \varepsilon^n \{\boldsymbol{\varepsilon}^n, \boldsymbol{\sigma}^n\}$. The first terms of these expansions are expressed in terms of \mathbf{u}^0 and $\boldsymbol{\chi}^1$ as

$$\begin{aligned} \boldsymbol{\varepsilon}^0(\mathbf{X}, \mathbf{x}) &= \text{sym}\{\nabla_{\mathbf{X}} \otimes \mathbf{u}^0(\mathbf{X})\} \\ &+ \text{sym}\{\nabla_{\mathbf{x}} \otimes \boldsymbol{\chi}^1(\mathbf{x})\} : (\nabla_{\mathbf{X}} \otimes \mathbf{u}^0(\mathbf{X})), \end{aligned} \quad (24)$$

$$\begin{aligned} \boldsymbol{\sigma}^0(\mathbf{X}, \mathbf{x}) &= \mathbf{C}(\mathbf{x}) : (\nabla_{\mathbf{x}} \otimes \boldsymbol{\chi}^1(\mathbf{x}) + \mathbf{1}^{(4s)}) \\ &: (\nabla_{\mathbf{X}} \otimes \mathbf{u}^0(\mathbf{X})), \end{aligned} \quad (25)$$

where $\text{sym}\{\nabla_{\mathbf{x}} \otimes \boldsymbol{\chi}^1\}$ stands for $(\partial \chi_{ikl}^1 / \partial x_j + \partial \chi_{jkl}^1 / \partial x_i) / 2$. Since $\boldsymbol{\chi}^1$ is periodic, the volume averages of $\boldsymbol{\varepsilon}^0$ and $\boldsymbol{\sigma}^0$ taken over U become

$$\begin{aligned} \langle \boldsymbol{\varepsilon}^0 \rangle_U(\mathbf{X}) &= \text{sym}\{\nabla_{\mathbf{X}} \otimes \mathbf{u}^0(\mathbf{X})\}, \\ \langle \boldsymbol{\sigma}^0 \rangle_U(\mathbf{X}) &= \overline{\mathbf{C}}^0 : \langle \boldsymbol{\varepsilon}^0 \rangle_U(\mathbf{X}), \end{aligned} \quad (26)$$

where $\overline{\mathbf{C}}^0$ is defined by Eq. (23). These volume averages correspond to the macrostrain and macrostress of the average-field theory. That is, if the strain and stress of $O(\varepsilon^0)$ are regarded as the microfields, the homogenization theory defines the macrofields as their volume averages, as does the average-field theory. Note that $\boldsymbol{\varepsilon}^0$ and $\boldsymbol{\sigma}^0$ are expressed in terms of $\langle \boldsymbol{\varepsilon}^0 \rangle_U$ and $\langle \boldsymbol{\sigma}^0 \rangle_U$ as

$$\begin{aligned} \boldsymbol{\varepsilon}^0(\mathbf{X}, \mathbf{x}) &= \langle \boldsymbol{\varepsilon}^0 \rangle(\mathbf{X}) + \text{sym}\{\nabla_{\mathbf{x}} \otimes \boldsymbol{\chi}^1(\mathbf{x})\} : \langle \boldsymbol{\varepsilon}^0 \rangle(\mathbf{X}), \\ \boldsymbol{\sigma}^0(\mathbf{X}, \mathbf{x}) &= \langle \boldsymbol{\sigma}^0 \rangle(\mathbf{X}) + (\mathbf{C}(\mathbf{X}) : (\text{sym}\{\nabla_{\mathbf{x}} \otimes \boldsymbol{\chi}^1(\mathbf{x})\} \\ &- \mathbf{1}^{(4s)}) - \overline{\mathbf{C}}^0) : \langle \boldsymbol{\varepsilon}^0 \rangle(\mathbf{X}). \end{aligned}$$

5. A hybrid micromechanics theory

While the homogenization theory is based on the singular perturbation of the microfields, the resulting fields of $O(\varepsilon^0)$ and their averages taken over U correspond to the microfields and the macrofields of the average-field theory; see Table 1 for the comparison of the field variables of $O(\varepsilon^0)$ with the field variables of the average-field theory.

Table 1
Comparison of average-field theory and homogenization theory

	Average field theory	Homogenization theory
Microdisplacement	\mathbf{u}	$\mathbf{u}^0 + \varepsilon \boldsymbol{\chi}^1 : (\nabla_X \otimes \mathbf{u}^0)$
Microstrain	$\boldsymbol{\epsilon} = \text{sym}\{\nabla_x \otimes \mathbf{u}\}$	$\boldsymbol{\epsilon}^0 = (\mathbf{1}^{(4s)} + \text{sym}\{\nabla_x \otimes \boldsymbol{\chi}^1\}) : \text{sym}\{\nabla_X \otimes \mathbf{u}^0\}$
Microstress	$\boldsymbol{\sigma} = \mathbf{C} : (\nabla_x \otimes \mathbf{u})$	$\boldsymbol{\sigma}^0 = \mathbf{C} : (\mathbf{1}^{(4s)} + \nabla_x \otimes \boldsymbol{\chi}^1) : (\nabla_X \otimes \mathbf{u}^0)$
Macrodisplacement	$\mathbf{U} = \int \phi_p \mathbf{u} \, dV$	\mathbf{u}^0
Macrostrain	$\mathbf{E} = \text{sym}\{\nabla_x \otimes \mathbf{U}\}$	$\langle \boldsymbol{\epsilon}^0 \rangle = \text{sym}\{\nabla_X \otimes \mathbf{u}^0\}$
Macrostress	$\boldsymbol{\Sigma} = \overline{\mathbf{C}} : \mathbf{E}$	$\langle \boldsymbol{\sigma}^0 \rangle = \overline{\mathbf{C}}^0 : \langle \boldsymbol{\epsilon}^0 \rangle$
Effective elasticity	$\overline{\mathbf{C}} = \mathbf{C}^M + f(\mathbf{C}^I - \mathbf{C}^M) : \mathbf{A}$	$\overline{\mathbf{C}}^0 = \langle \mathbf{C} : (\mathbf{1}^{(4s)} + \nabla_x \otimes \boldsymbol{\chi}^1) \rangle$

There are, however, two major differences between these two theories. The first difference is the modeling of the microstructure: the homogenization theory uses a unit cell of the periodic structure, while the average-field theory considers a representative volume element of a statistically homogeneous body. The second difference is that the homogenization theory is able to treat the macro–micro relations more rigorously, allowing higher-order terms in the singular perturbation expansion. These differences are not *essential*, i.e., the homogenization theory can be applied to materials with a non-periodic microstructure and higher order terms can be still computed with the aid of suitable microstructure models using the average-field theory. In this section, we propose a micromechanics theory which is a hybrid of the homogenization and average-field theories. Since tensors of higher order appear, index notation is mainly used in this section; in particular, ∇_X and ∇_x are replaced by $D_i \equiv \partial/\partial X_i$ and $d_i \equiv \partial/\partial x_i$, respectively.

5.1. More general modeling of microstructure

We consider an elasticity tensor field $\mathbf{C} = \mathbf{C}(\mathbf{x})$ which is not necessarily periodic. The singular perturbation of \mathbf{u}^ε , Eq. (19), is still applicable, and the assumptions of $u_i^0 = \chi_{im}^0 u_m^0(\mathbf{X})$ and $u_i^1 = \chi_{imp}^1(\mathbf{x})(D_p u_m^0(\mathbf{X}))$ make terms of $O(\varepsilon^{-2})$ and $O(\varepsilon^{-1})$ vanish, if $\chi_{ij}^0 = \delta_{ij}$ and $\boldsymbol{\chi}^1$ satisfies Eq. (21).

Furthermore, assuming that \mathbf{u}^2 is given by $u_i^2 = \chi_{impq}^2(D_p D_q u_m^0)$, where $\boldsymbol{\chi}^2$ is a fourth-order tensor depending only on \mathbf{x} , we rewrite terms of $O(\varepsilon^0)$ in Eq. (20) as follows:

$$\overline{\mathbf{C}}_{ijkl}^{0r} D_i D_l u_k^0(\mathbf{X}) + R_j^0(\mathbf{X}, \mathbf{x}), \tag{*}$$

where, at this stage, $\overline{\mathbf{C}}^{0r}$ is as yet an arbitrary fourth-order tensor, and \mathbf{R}^0 is defined as

$$R_j^0(\mathbf{X}, \mathbf{x}) = \left(d_i \left(C_{ijkl}(\mathbf{x})(d_i \chi_{kmpq}^2(\mathbf{x}) + \chi_{kmq}^1(\mathbf{x})\delta_{lp}) \right) + C_{pjkl}(\mathbf{x})(d_i \chi_{kmq}^1(\mathbf{x}) + \chi_{km}^0 \delta_{lq}) - \overline{\mathbf{C}}_{pjm}^0 \right) \times (D_p D_q u_m^0(\mathbf{X})). \tag{27}$$

The first term in (*) yields a governing equation for \mathbf{u}^0 and the second term, R_j^0 , is a residue of this governing equation.

It is possible to enforce $\mathbf{R}^0 = 0$ and to satisfy Eq. (20) up to $O(\varepsilon^0)$ for any arbitrary $\overline{\mathbf{C}}^{0r}$, since $\boldsymbol{\chi}^2$ can be determined such that \mathbf{R}^0 vanishes. According to the average-field theory, however, the most suitable $\overline{\mathbf{C}}^r$ is probably given by taking the volume average of $C_{ijpq}(d_q \chi_{pkl}^1 + \chi_{pk}^0 \delta_{lq})$, over a domain in which $\boldsymbol{\chi}^1$ is defined.

Let V be a domain in which $\boldsymbol{\chi}^1$ is defined. Although V is not necessarily a unit cell of a periodic structure, we seek to determine $\boldsymbol{\chi}^1$ or $\overline{\mathbf{C}}^{0r}$ which relates the average strain to the average strain energy as well as the average stress, independently

⁷ Here, $\chi_{ik}^0 = \delta_{ik}$ is introduced to make the expression of \mathbf{u}^0 consistent with other \mathbf{u}^n 's.

⁸ From mathematical point of view, the most suitable $\overline{\mathbf{C}}^{0r}$ can be defined by minimizing a suitable measure of the perturbation error of $O(\varepsilon^1)$.

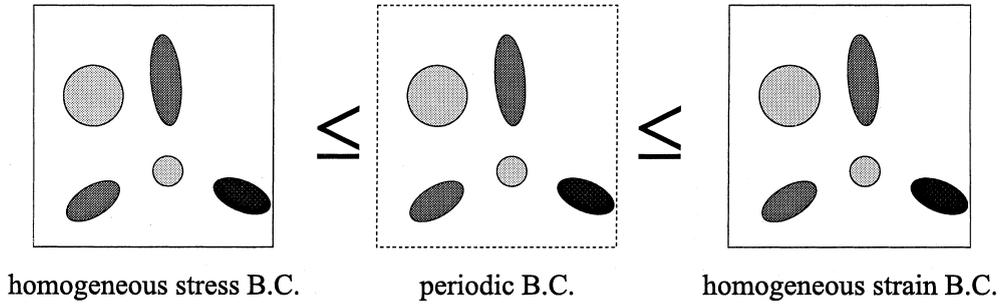


Fig. 5. Unit cell used in hybrid micromechanics theory.

of the boundary conditions prescribed on ∂V . According to the universal inequalities (17), the following two inequalities hold

$$\int_V \epsilon^{0\Sigma} : C : \epsilon^{0\Sigma} dV_x \leq \int_V \epsilon^{0G} : C : \epsilon^{0G} dV_x \leq \int_V \epsilon^{0E} : C : \epsilon^{0E} dV_x, \quad (28)$$

where ϵ^{0E} , ϵ^{0G} , and $\epsilon^{0\Sigma}$, respectively, are the strain fields of $O(\epsilon^0)$ when homogeneous strain, general, and homogeneous stress boundary conditions are prescribed on ∂V in such a manner that they produce the same average strain. These χ^{1E} , χ^{1G} , and $\chi^{1\Sigma}$ are given by

$$\epsilon^{0(\cdot)}(X, x) = \text{sym}\{(\nabla_x \otimes \chi^{1(\cdot)}(x) + \mathbf{1}^{(4s)}) : (\nabla_X \otimes \mathbf{u}^0(X))\},$$

and give the micro-scopic strain whose volume average coincides with $\text{sym}\{\nabla_X \otimes \mathbf{u}^0\}$, i.e.,

$$\langle \text{sym}\{(\nabla_x \otimes \chi^{1(\cdot)} + \mathbf{1}^{(4s)}) : (\nabla_X \otimes \mathbf{u}^0)\} \rangle_V(X) = \text{sym}\{\nabla_X \otimes \mathbf{u}^0(X)\}. \quad (29)$$

Hence, the average response of V does not depend on the prescribed boundary conditions, if⁹ value of average strain energy of V under the homogeneous strain boundary conditions, $\langle e^E \rangle_V$, is close to

the value of the average strain energy under the homogeneous stress boundary conditions, $\langle e^\Sigma \rangle_V$, i.e.,

$$\frac{\langle e^E \rangle_V - \langle e^\Sigma \rangle_V}{\langle e^E \rangle_V} \ll 1, \quad (30)$$

where

$$\langle e^{(\cdot)} \rangle_V = \langle \frac{1}{2} \epsilon^{0(\cdot)} : C : \epsilon^{0(\cdot)} \rangle_V. \quad (31)$$

The effective elasticity tensor, \bar{C}^{0r} , can now be uniquely determined as

$$\bar{C}^{0r} \approx \langle C : (\nabla_x \otimes \chi^{1E} + \mathbf{1}^{(4s)}) \rangle_V \quad (\text{or } \langle C : (\nabla_x \otimes \chi^{1\Sigma} + \mathbf{1}^{(4s)}) \rangle_V). \quad (32)$$

The effective elasticity tensor, \bar{C}^0 , which is given by Eq. (23), corresponds to a case when periodic boundary conditions are prescribed on the boundary of a parallelepiped $V = U$; see Fig. 5. This effective elasticity tensor is bounded by two effective elasticity tensors, $\langle C : (\nabla_x \otimes \chi^{1E} + \mathbf{1}^{(4s)}) \rangle_V$ and $\langle C : (\nabla_x \otimes \chi^{1\Sigma} + \mathbf{1}^{(4s)}) \rangle_V$, which are determined when homogeneous strain and stress boundary conditions are prescribed on the parallelepiped U .

For a given (constant) average strain, $\langle \epsilon^0 \rangle_V = \text{sym}\{\nabla_X \otimes \mathbf{u}^0\}$, the boundary conditions for χ^{1E} is prescribed as $\chi^{1E} = 0$ on ∂V . Boundary conditions for $\chi^{1\Sigma}$, however, are not easily defined; zero traction boundary conditions, $\mathbf{v} \cdot (C : (\nabla_x \otimes \chi^{1\Sigma})) = 0$, are not suitable since the resulting $\chi^{1\Sigma}$ does not satisfy Eq. (29). Taking advantage of the

⁹ These two boundary data produce fields satisfying Eq. (29), and hence the average strains are the same.

linearity, however, we can determine $\chi^{1\Sigma}$ using the solution for the homogeneous stress boundary conditions. Indeed, let $\mathbf{u}^\Sigma = \mathbf{u}^\Sigma(\mathbf{x}; \Sigma)$ be the displacement field when V is subjected to $\mathbf{t} = \mathbf{v} \cdot \Sigma$ on ∂V , where Σ is constant. The volume average of the associated strain, $\langle \epsilon^\Sigma \rangle_V = \langle \text{sym}\{\nabla_{\mathbf{x}} \otimes \mathbf{u}^\Sigma\} \rangle_V$, is linearly related to the prescribed stress, Σ , which is the same as the average stress. Hence, the inverse of a fourth-order tensor which relates Σ to $\langle \epsilon^\Sigma \rangle_V$ is the effective elasticity tensor, and $\chi^{1\Sigma}$ is given by

$$\chi^{1\Sigma}(\mathbf{x}) : \langle \epsilon^\Sigma \rangle_V = \mathbf{u}^\Sigma(\mathbf{x}; \Sigma) - \mathbf{x} \cdot \langle \epsilon^\Sigma \rangle_V.$$

This $\chi^{1\Sigma}$ satisfies Eq. (29), if Σ is chosen such that $\langle \epsilon^\Sigma \rangle_V = \langle \epsilon^0 \rangle_V$ or $\text{sym}\{\nabla_{\mathbf{x}} \otimes \mathbf{u}^0\}$.

5.2. Treatment of higher-order terms

It is of interest to examine the effects of the higher order terms; in particular, the second-order terms which, as shown later, are associated with the effects of the macroscopic strain gradients. It should be noted that when the material is linearly elastic, higher order terms in the perturbation expansion may not be significant, since the volume averages of these terms taken over V vanish. In non-linear cases, however, there are cases when such higher order terms make significant contributions.

The homogenization theory usually assumes that the n th order term, u_i^n , is given by

$$u_i^n(\mathbf{X}, \mathbf{x}) = \chi_{i m p_1 p_2 \dots p_n}^n(\mathbf{x}) D_{p_1} D_{p_2} \dots D_{p_n} u_m^0(\mathbf{X}),$$

and derives a boundary-value problem for χ^n from the terms of $O(\epsilon^{n-2})$ in Eq. (20) using periodic boundary conditions; see Appendix B for a brief summary of the treatment of such higher order terms in the homogenization theory. For instance, when $u_i^2 = \chi_{i m p q}^2(\mathbf{x}) D_p D_q u_m^0(\mathbf{X})$ is included, the terms of $O(\epsilon^1)$ are written as

$$\bar{C}_{i j m p q}^1 D_i D_p D_q u_m^0(\mathbf{X}) + R_j^1(\mathbf{X}, \mathbf{x}),$$

where \bar{C}^1 is

$$\bar{C}_{i j m p q}^1 = \langle C_{i j k l} (d_l \chi_{k m p q}^2 + \chi_{k m p}^1 \delta_{l q}) \rangle_U, \tag{33}$$

and R^1 is similar in form to R^0 . In order to satisfy Eq. (20) up to $O(\epsilon^1)$, \mathbf{u}^0 must satisfy

$$\bar{C}_{i j k l}^0 D_i D_l u_k^0(\mathbf{x}) + \epsilon \bar{C}_{i j k l m}^1 D_i D_l D_m u_k^0(\mathbf{x}) = 0 \text{ in } B.$$

The homogenization theory takes another (regular) perturbation expansion for \mathbf{u}^0 ,

$$\mathbf{u}^0(\mathbf{X}) \approx \mathbf{U}^0(\mathbf{X}) + \epsilon \mathbf{U}^1(\mathbf{X}) + \dots, \tag{34}$$

and obtains a set of governing equations for \mathbf{U}^0 and \mathbf{U}^1 as follows:

$$\bar{C}_{i j k l}^0 D_i D_l U_k^0(\mathbf{X}) = 0 \text{ in } B, \tag{35}$$

$$\bar{C}_{i j k l}^0 D_i D_l U_k^1(\mathbf{X}) + \bar{C}_{i j k l m}^1 D_i D_l D_m U_k^0(\mathbf{X}) = 0 \text{ in } B. \tag{36}$$

Since $\mathbf{u}^\epsilon \approx \mathbf{u}^0 + \epsilon \mathbf{u}^1$ is replaced by $\mathbf{U}^0 + \epsilon(\mathbf{U}^1 + \chi^1 : (\nabla_{\mathbf{x}} \otimes \mathbf{U}^0))$, the boundary conditions for \mathbf{U}^0 and \mathbf{U}^1 are $\mathbf{U}^0 = \mathbf{u}^0$ and $\mathbf{U}^1 = 0$ on ∂B . Hence, once \mathbf{U}^0 is obtained by solving Eq. (35), \mathbf{U}^1 is determined by solving Eq. (36) with $\mathbf{U}^1 = 0$ on ∂U .

As shown in the preceding subsection, the periodicity of \mathbf{C} is not essential. The governing equations for the higher order terms, χ^n s, remain the same if the domain V is used as a microstructure model. For instance, the governing equation for χ^2 is derived from $\mathbf{R}^0 = 0$. In view of Eq. (27), they are expressed in terms of χ^1 as follows

$$d_i \left(C_{i j k l}(\mathbf{x}) d_l \chi_{k m p q}^2(\mathbf{x}) \right) + \left(d_i (C_{i j k p}(\mathbf{x}) \chi_{k m q}^1(\mathbf{x})) + C_{p j k l}(\mathbf{x}) (d_l \chi_{k m q}^1(\mathbf{x}) + C_{p j m q}(\mathbf{x}) - \bar{C}_{p j m q}^{0'}) \right) = 0. \tag{37}$$

Note that \bar{C}^0 is replaced by $\bar{C}^{0'}$ which is given by Eq. (32).

If m, p , and q are fixed, $\chi_{k m p q}^2$ is the displacement field of V when body forces are prescribed by the terms in the parenthesis. Since V is chosen such that the dependence of the average response on prescribed boundary conditions is negligibly small, we can determine $\chi_{k m p q}^2$ assuming either zero displacements ($\chi_{k m n p q}^2 = 0$) or zero tractions ($n_i C_{i j k l} d_l \chi_{k m p q}^2 = 0$) on ∂V . Such χ^{2E} or $\chi^{2\Sigma}$ replaces \bar{C}^1 in Eq. (33) which is computed for a unit cell;

for instance, when zero displacement boundary conditions are used,

$$\bar{C}_{ijmpq}^{1'} = \langle C_{ijkl}(\delta_l \chi_{kmpq}^{2E} + \chi_{kmp}^{1E} \delta_{lq}) \rangle_V. \quad (38)$$

Here, superscript E emphasizes that χ^1 and χ^2 are for zero displacement boundary conditions.

Once $\bar{C}^{0'}$ and $\bar{C}^{1'}$ are determined, the governing equations for U^0 and U^1 are rewritten by replacing \bar{C}^0 and \bar{C}^1 with $\bar{C}^{0'}$ and $\bar{C}^{1'}$, respectively. That is,

$$\bar{C}_{ijkl}^{0'} D_i D_l U_k^0(\mathbf{X}) = 0 \quad \text{in } B, \quad (39)$$

$$\bar{C}_{ijkl}^{0'} D_i D_l U_k^1(\mathbf{X}) + \bar{C}_{ijklm}^{1'} D_i D_l D_m U_k^0(\mathbf{X}) = 0 \quad \text{in } B. \quad (40)$$

While it is possible to solve these equations in a recursive manner and to determine $u^e \approx U^0 + \varepsilon(U^1 + \chi^1 : (\nabla_x \otimes U^0))$, we derive instead a governing equation for u^e which accounts for the effects of higher order terms. To this end, assuming that $\bar{C}^{0'}$ is invertible, we first rewrite the left side of Eq. (40) as

$$D_i \bar{C}_{ijhp}^{0'} D_t (\delta_{pt} U_h^1 + ((\bar{C}^{0'})^{-1} : \bar{C}^{1'})_{hprst} (D_s U_r^0)).$$

We seek to obtain a suitable function \mathbf{B} which satisfies $D_i (\bar{C}_{ijhp}^{0'} D_t B_{hpt}) = 0$. This \mathbf{B} gives U^1 as $\delta_{pt} U_h^1 = B_{hpt} - ((\bar{C}^{0'})^{-1} : \bar{C}^{1'})_{hprst} D_s U_r^0$, or, summing over p and t ,

$$U_i^1(\mathbf{X}) = \frac{1}{3} (B_{ipp}(\mathbf{X}) - ((\bar{C}^{0'})^{-1} : \bar{C}^{1'})_{ipklp} (D_l U_k^0(\mathbf{X}))). \quad (41)$$

According to the standard procedure of the homogenization theory, \mathbf{B} should be determined such that the boundary conditions prescribed for U^1 are satisfied. However, according to the average-field theory which regards a macroscopic field variable as the local average of the corresponding microscopic variable, it is more natural to locally relate U^1 to the gradient of U^0 , neglecting \mathbf{B} in Eq. (41). That is, to set

$$U_i^1(\mathbf{X}) \approx \Xi_{ikl} (D_l U_k^0(\mathbf{X})), \quad (42)$$

where Ξ is a third-order constant tensor given by

$$\Xi_{ikl} = ((\bar{C}^{0'})^{-1} : (\bar{C}^{1'}))_{ipklp} = (\bar{C}^{0'})_{ipmn}^{-1} \bar{C}_{mnklp}^{1'}. \quad (43)$$

Since $\bar{C}^{0'}$ and $\bar{C}^{1'}$ are determined from χ^1 and χ^2 , this Ξ can be explicitly determined once the microstructure model is established.

In view of Eq. (42), we obtain a relation between u^e and U^0 , which accounts for the second-order terms, i.e.,

$$u_i^e(\mathbf{X}) \approx U_i^0(\mathbf{X}) + \varepsilon(\Xi_{ikl} + \chi_{ikl}^1(\mathbf{x})) (D_l U_k^0(\mathbf{X})) + \dots \quad (44)$$

It is straightforward to obtain the inverse relation between u^e and U^0 up to $O(\varepsilon)$, as

$$U_i^0(\mathbf{X}) \approx u_i^e(\mathbf{X}) - \varepsilon(\Xi_{ikl} + \chi_{ikl}^1(\mathbf{x})) (D_l u_k^e(\mathbf{X})) + \dots \quad (45)$$

In this equation, χ^1 is the only term which changes within a micro-length scale, or the only function which depends on \mathbf{x} . If, say, the volume average of χ^1 is taken over V , then, the right side of this equation is approximated by $u_i^e - \varepsilon(\Xi_{ikl} + \langle \chi_{ikl}^1 \rangle) (D_l u_k^e)$, a function of \mathbf{X} only. Hence, the following equations are obtained from Eq. (39):

$$D_i \left(\bar{C}_{ijkl}^{0'} D_l u_k^e(\mathbf{X}) + \varepsilon \bar{C}_{ijklmn}^{1'} D_l D_m u_k^e(\mathbf{X}) \right) = 0 \quad \text{in } B, \quad (46)$$

where \bar{C} is defined by

$$\bar{C}_{ijklm}^{1'} = -\bar{C}_{ijpl}^{0'} (\Xi_{pkm} + \langle \chi_{pkm}^1 \rangle_V), \quad (47)$$

and satisfies the symmetry property,

$$\bar{C}_{ijklm}^{1'} = \bar{C}_{ijkml}^{1'} = \bar{C}_{ijlkm}^{1'}, \quad \bar{C}_{ijklm}^{1'} = \bar{C}_{jiklm}^{1'}.$$

While $\varepsilon \bar{C}_{ijklm}^{1'} D_l D_m u_k^e$ in Eq. (46) are mathematically derived from the perturbation analysis, these terms can be interpreted as stress due to the strain gradient; the left side of Eq. (46) is rewritten as $D_i \sigma_{ij}^e$, where σ_{ij}^e is given by

$$\sigma_{ij}^e(\mathbf{X}) = \bar{C}_{ijkl}^{1'} \epsilon_{kl}^e(\mathbf{X}) + \varepsilon \bar{C}_{ijklm}^{1'} \epsilon_{klm}^{e'}(\mathbf{X}). \quad (48)$$

¹⁰ By definition, Ξ satisfies the symmetry property, $\Xi_{ikl} = \Xi_{ilk}$.

Here, ϵ_{ij}^e is the strain associated with \mathbf{u}^e ($\text{sym}\{D_i u_j^e\}$), and ϵ_{ijk}^e is the gradient of the strain given by

$$\epsilon_{ijk}^e(\mathbf{X}) = \frac{1}{3} \left(D_i D_j u_k^e(\mathbf{X}) + D_j D_k u_i^e(\mathbf{X}) + D_k D_i u_j^e(\mathbf{X}) \right). \quad (49)$$

Fig. 6 summarizes the hybrid micromechanics theory presented in this section.

It should be noted that both $\bar{\mathbf{C}}^{0'}$ and $\bar{\mathbf{C}}$ are fully determined from the microstructure model. The effects of $\bar{\mathbf{C}}$, however, can be neglected as

they are proportional to ϵ . In addition to this, $\bar{\mathbf{C}}$ is small for linear problems, because: (1) Ξ is small since it gives the overall displacement when a linearly varying strain field with zero volume average is prescribed; and (2) $\langle \chi^1 \rangle_V$ is small since it gives the average displacement when the microstructure model is subjected to zero displacements (or traction) boundary conditions. Therefore, it is concluded that the effects of $\bar{\mathbf{C}}$ or the strain gradient can be omitted unless the microstructure model is non-linear and large strain gradients are presented.

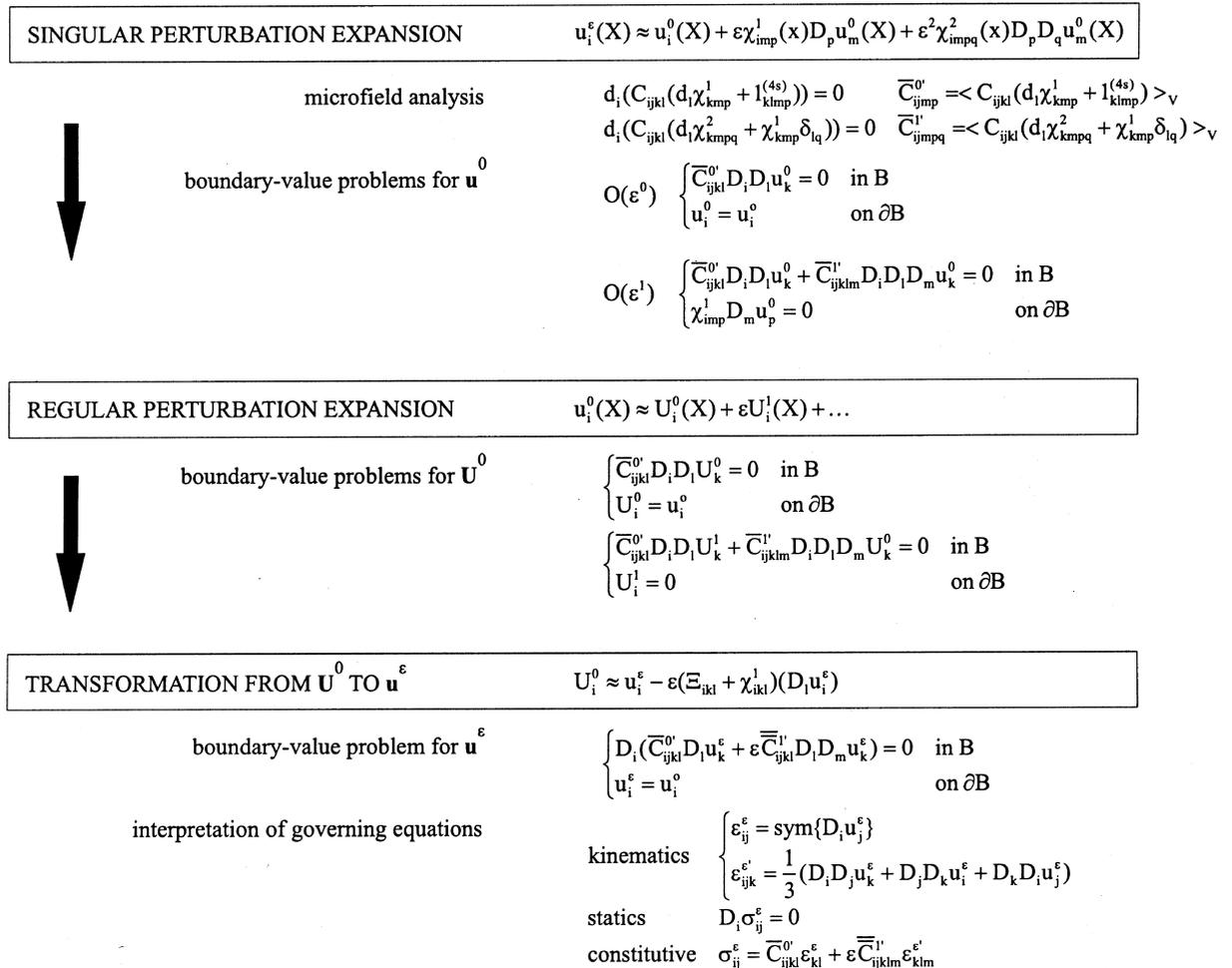


Fig. 6. Summary of hybrid micromechanics theory.

6. Periodic boundary conditions

When the microstructure model V is given, there arises the question of what boundary conditions should be used to determine the effective moduli of the first and higher orders. As shown in the preceding section, we may use the homogeneous stress and strain boundary conditions such that the solutions of the resulting macrofield equations can overestimate or underestimate¹¹ macroscopic responses which are obtained by using other effective moduli, since these boundary conditions provide upper and lower bounds for all possible effective moduli. If the difference of these upper and lower bounds are large, however, we may use the periodic boundary conditions. This is because they provide the effective moduli which represent those obtained by using a certain class of boundary conditions. This property of the periodic boundary conditions is shown in this section.

For simplicity, consider a cubic representative volume element, denoted by U , with the edge length 2π . Let $\bar{\mathbf{u}}^P$ and $\bar{\mathbf{t}}^P$ be the surface displacement and traction when periodic boundary conditions are prescribed, and the resulting average strain, stress, and strain energy are denoted by \mathbf{E} , $\mathbf{\Sigma}$, and $\langle e^P \rangle_U$. Due to the uniqueness of the solution, displacement boundary conditions of $\mathbf{u} = \bar{\mathbf{u}}^P$ on ∂U or traction boundary conditions of $\mathbf{t} = \bar{\mathbf{t}}^P$ on ∂U yield the same response when the periodic boundary conditions are prescribed.

First, consider a disturbance in displacement boundary conditions, $\mathbf{u} = \bar{\mathbf{u}}^P + d\bar{\mathbf{u}}$ on ∂U . The strain energy due to $d\bar{\mathbf{u}}$ is expressed as

$$\langle e^P \rangle_U + \langle de \rangle_U + \langle d^2e \rangle_U,$$

where $\langle de \rangle_U$ and $\langle d^2e \rangle_U$ are functions of $d\bar{\mathbf{u}}$, defined by

$$\langle de \rangle_U(d\bar{\mathbf{u}}) = \frac{1}{U} \int_{\partial U} \bar{\mathbf{t}}^P \cdot d\bar{\mathbf{u}} \, dS, \tag{50}$$

$$\langle d^2e \rangle_U(d\bar{\mathbf{u}}) = \frac{1}{2U} \int_{\partial U} \mathbf{t}(d\bar{\mathbf{u}}) \cdot d\bar{\mathbf{u}} \, dS, \tag{51}$$

with $\mathbf{t}(d\bar{\mathbf{u}})$ being the surface tractions when the boundary conditions are $\mathbf{u} = d\bar{\mathbf{u}}$ on ∂U . Due to the periodicity of $\bar{\mathbf{t}}^P$, the functional $\langle de \rangle_U$ vanishes for the disturbance displacement of the following form

$$d\bar{\mathbf{u}}^P(\mathbf{x}) = \sum_{m_1, m_2, m_3 = -M}^M d\mathbf{u}_m \exp(i\mathbf{m} \cdot \mathbf{x}) \text{ on } \partial U,$$

where $d\mathbf{u}_m$ s are arbitrary constants and M is an arbitrary number. Indeed, at, say, $(-\pi, x_2, x_3)$ and (π, x_2, x_3) on ∂U , the integrand satisfies

$$(\bar{\mathbf{t}}^P \cdot \bar{\mathbf{u}}^P)(-\pi, x_2, x_3) = (\bar{\mathbf{t}}^P \cdot \bar{\mathbf{u}}^P)(\pi, x_2, x_3),$$

since the stress and displacement take the same value due to the periodicity but the unit normals are in the opposite direction; see Nemat-Nasser and Hori (1993), Section 12. This $d\bar{\mathbf{u}}^P$ does not change the average strain since it is periodic. It follows from $\langle d^2e \rangle_U > 0$ that the displacement boundary conditions of $\mathbf{u} = \bar{\mathbf{u}}^P$ on ∂U yield the minimum strain energy among the class of displacement boundary conditions of $\mathbf{u} = \bar{\mathbf{u}}^P + d\bar{\mathbf{u}}^P$ on ∂U .

Next, consider a class of traction boundary conditions which disturb traction boundary conditions, $\mathbf{t} = \bar{\mathbf{t}}^P$ on ∂U . These boundary conditions produce the same field variables as the periodic boundary conditions. Let $d\bar{\mathbf{t}}$ be a disturbance, and $\mathbf{t} = \bar{\mathbf{t}}^P + d\bar{\mathbf{t}}$ on ∂U be the traction boundary conditions. The strain energy is given as $\langle e^P \rangle_U + \langle de' \rangle_U + \langle d^2e' \rangle_U$, where

$$\langle de' \rangle_U(d\bar{\mathbf{t}}) = \frac{1}{U} \int_{\partial U} d\bar{\mathbf{t}} \cdot \bar{\mathbf{u}} \, dS, \tag{52}$$

$$\langle d^2e' \rangle_U(d\bar{\mathbf{t}}) = \frac{1}{2U} \int_{\partial U} d\bar{\mathbf{t}} \cdot \mathbf{u}(d\bar{\mathbf{t}}) \, dS, \tag{53}$$

with $\mathbf{u}(d\bar{\mathbf{t}})$ being the surface displacements when the boundary conditions are $\mathbf{t} = d\bar{\mathbf{t}}$ (rigid-body motion is excluded). The periodicity of $\bar{\mathbf{u}}^P - \mathbf{x} \cdot \mathbf{E}$ leads to $\langle de' \rangle_U = 0$ for $d\bar{\mathbf{t}}$ of the following form

$$d\bar{\mathbf{t}}^P(\mathbf{x}) = \mathbf{v}(\mathbf{x}) \cdot \left(\sum_{m_1, m_2, m_3 = -M}^M d\boldsymbol{\sigma}_m \exp(i\mathbf{m} \cdot \mathbf{x}) \right) \text{ on } \partial U,$$

where $d\boldsymbol{\sigma}_m$ s are arbitrary except for $d\boldsymbol{\sigma}_0 = 0$. This $d\bar{\mathbf{t}}^P$ does not change the average stress. Hence, the

¹¹ See Munashinghe et al. (1996).

boundary condition $\mathbf{t} = \bar{\mathbf{t}}^P$ on ∂U yields the minimum strain energy for this class of traction-boundary conditions. Equivalently, $\mathbf{t} = \bar{\mathbf{t}}^P$ yields the maximum strain energy of the class of traction boundary conditions $\mathbf{t} = \boldsymbol{\Sigma}' + \bar{\mathbf{t}}^P$ on ∂U , where $\boldsymbol{\Sigma}'$ is chosen such that the resulting average strain is \mathbf{E} .

Now, denote by $\langle e^E \rangle_U$ and $\langle e^\Sigma \rangle_U$ the average strain energy due to the homogeneous strain and stress boundary conditions which produce the same average strain, \mathbf{E} . It then follows from the two universal theorems that for the above arbitrarily disturbed boundary conditions which produce the average strain \mathbf{E} , the resulting average strain energy is bounded as follows

$$\begin{aligned} \langle e^\Sigma \rangle_U &\leq \langle e^P \rangle_U + \langle d^2 e' \rangle (d\bar{\mathbf{t}}^P) \leq \langle e^P \rangle_U \\ &\leq \langle e^P \rangle_U + \langle d^2 e \rangle (d\bar{\boldsymbol{\mu}}^P) \leq \langle e^E \rangle_U; \end{aligned} \quad (54)$$

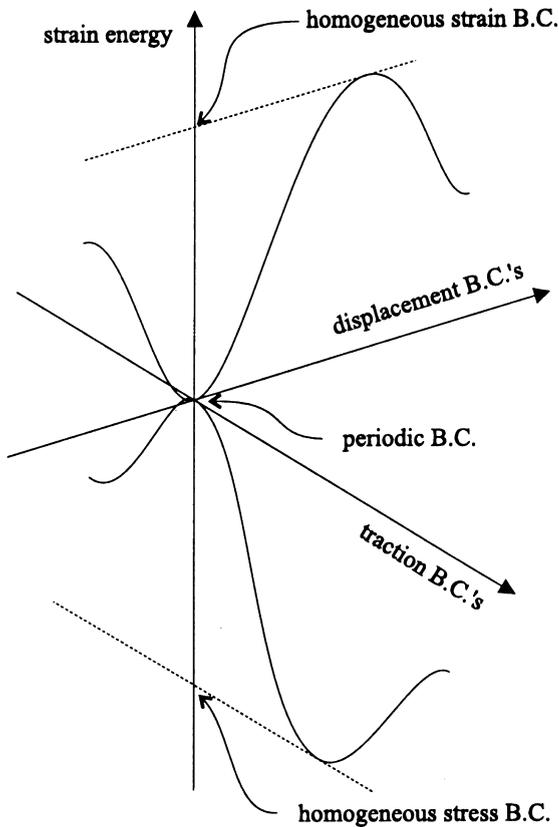


Fig. 7. Dependence of strain energy on boundary data.

see Fig. 7 for the schematic view of these inequalities. In this sense, we regard the periodic boundary conditions as the boundary conditions that represent¹² the two classes of the boundary conditions, $\mathbf{u} = \bar{\mathbf{u}}^P + d\bar{\boldsymbol{\mu}}^P$ and $\mathbf{t} = \bar{\mathbf{t}}^P + d\bar{\boldsymbol{\mu}}^P$ on ∂U .

7. Concluding remarks

It is shown that the two micromechanics theories, the average-field theory and the homogenization theory, can be related to each other, even though they are based on different concepts. In particular, the first order terms in the expanded strain and stress fields of the homogenization theory correspond to the average strain and stress considered in the average-field theory. Taking advantage of this correspondence, we combine the two theories to obtain a hybrid micromechanics theory, which is applicable to a representative volume element, while, at the same time, it allows us to compute the overall properties more accurately than possible with the average-field theory. The new resulting field equations for the macrodisplacement in this hybrid theory include the effects of the macrostrain gradient in a natural manner.

Appendix A. Strain concentration of average-field theory

Suppose that V is a multi-phase composite, consisting of N phases, each with a distinct elasticity tensor \mathbf{C}^α , and a matrix phase of the elasticity tensor \mathbf{C}^M . If V is statistically homogeneous, and $\langle \boldsymbol{\epsilon}^E : \mathbf{C} : \boldsymbol{\epsilon}^E \rangle_V - \langle \boldsymbol{\epsilon}^\Sigma : \mathbf{C} : \boldsymbol{\epsilon}^\Sigma \rangle_V$ is negligibly small for the same average strain $\langle \boldsymbol{\epsilon}^E \rangle = \langle \boldsymbol{\epsilon}^\Sigma \rangle$, the effective elasticity tensor $\bar{\mathbf{C}}$ is determined by considering a response of V subjected to, say, the homogeneous strain boundary conditions. By

¹² The strict mean of the strain energy is defined as $(\langle e^E \rangle_U + \langle e^\Sigma \rangle_U)/2$. Depending on the microstructure, $\langle e \rangle_U$ precisely satisfies $\langle e \rangle_U = (\langle e^E \rangle_U + \langle e^\Sigma \rangle_U)/2$, though this equality does not always hold.

definition, $\bar{\mathbf{C}}$ gives the relation between the average strain and stress, and the following exact equality holds

$$(\bar{\mathbf{C}} - \mathbf{C}^M) : \langle \boldsymbol{\epsilon} \rangle_V = \sum_{\alpha=1}^N f^\alpha (\mathbf{C}^\alpha - \mathbf{C}^M) : \langle \boldsymbol{\epsilon} \rangle_\alpha,$$

where f^α and $\langle \cdot \rangle_\alpha$ are the volume fraction and the volume average of the α -th phase. Hence, if the strain concentration of the α th phase is given by $\langle \boldsymbol{\epsilon} \rangle_\alpha = \mathbf{A}^\alpha : \langle \boldsymbol{\epsilon} \rangle_V$, then the effective elasticity tensor becomes

$$\bar{\mathbf{C}} = \mathbf{C}^M + \sum_{\alpha=1}^N f^\alpha (\mathbf{C}^\alpha - \mathbf{C}^M) : \mathbf{A}^\alpha.$$

Appendix B. Higher order terms in homogenization theory

If $u_m^n (= \chi_{mkp_1 \dots p_n}^n (\mathbf{D}_{p_1} \dots \mathbf{D}_{p_n} u_m^0))$ s are used, terms of $O(\varepsilon^n)$ in the singular perturbation expansion of the governing equation become

$$\bar{\mathbf{C}}_{ijm p_1 \dots p_{n+1}}^n \mathbf{D}_i \mathbf{D}_{p_1} \dots \mathbf{D}_{p_{n+1}} u_m^0 + \mathbf{R}_j^n,$$

where

$$\begin{aligned} \bar{\mathbf{C}}_{ijm p_1 \dots p_{n+1}}^n &= \langle C_{ijkl} (\mathbf{d}_i \chi_{kmp_1 \dots p_{n+1}}^{n+1} + \chi_{kmp_1 \dots p_n}^n \delta_{lp_{n+1}}) \rangle_U \\ \mathbf{R}_j^n &= \left\{ \mathbf{d}_i \left\{ C_{ijkl} (\mathbf{d}_l \chi_{kmp_1 \dots p_{n+2}}^{n+2} + \chi_{kmp_1 \dots p_{n+1}}^{n+1} \delta_{lp_{n+2}}) \right\} \right. \\ &\quad + \delta_{ip_{n+2}} \left\{ C_{ijkl} (\mathbf{d}_l \chi_{kmp_1 \dots p_{n+1}}^{n+1} + \chi_{kmp_1 \dots p_n}^n \delta_{lp_{n+1}}) \right\} \\ &\quad \left. + \delta_{ip_{n+2}} \bar{\mathbf{C}}_{pn+2, j p_1 \dots p_{n+1}}^n \right\} \mathbf{D}_{p_1} \dots \mathbf{D}_{p_{n+2}} u_m^0. \end{aligned}$$

The $(n + 4)$ th order tensor $\bar{\mathbf{C}}^n$ gives a governing equation for u^0 up to $O(\varepsilon^n)$, i.e.,

$$\sum_{m=0}^n \varepsilon^m \bar{\mathbf{C}}_{ijm p_1 \dots p_{m+1}}^m \mathbf{D}_i \mathbf{D}_{p_1} \dots \mathbf{D}_{p_{m+1}} u_m^0 = 0.$$

Terms in the parenthesis of the right side of \mathbf{R}^n s equations yield a governing equation for χ^{n+2} , and recursive formulae for χ^n s are naturally obtained. It is easily seen that χ^n s have symmetry properties for their suffices; for instance, χ^1 satisfies

$\chi_{mkp}^1 = \chi_{mpk}^1$ as it gives a displacement component in the x_m -direction when an (x_k, x_p) -component of macrostrain is presented. Similarly, χ^2 satisfies $\chi_{mkpq}^2 = \chi_{mkqp}^2 = \chi_{mpkq}^2$.

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