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A Relation Between Multiple-Scattering Theory and Micromechanical Models of Effective Thermoelastic Properties

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Abstract: A relation between multiple-scattering theory and micromechanical models of effective elastic material properties of heterogeneous materials has been established within a unified theoretical framework, and exemplified on three important approximations, the average t-matrix (or Mori–Tanaka), symmetric self-consistency (coherent potential), and asymmetric self-consistency approximations. © 1996 Elsevier Science Limited and Techna S.r.l.

1 INTRODUCTION

There has been much work on the description and prediction of the structure–property relationships of heterogeneous materials (HM), such as polycrystals, composites, and porous materials, for over half a century, as such materials have found many structural and functional applications (see, for example, Refs 1–3). Theoretically, the problem of determining the effective properties of HM can be attacked in several different ways. Among the more interesting ones are multiple-scattering theory[4] and micromechanical theory.[5] The multiple-scattering theory invokes theoretical methods known from quantum mechanics and solid-state physics. The scattering theory, often called effective-medium theory, has been widely employed to determine the structure–physical property relationships of HM,[3] and has been used mainly by materials physicists. Recently, this method has also been applied to the calculation of the effective elastic,[6] thermoelastic,[7] and elastoplastic[8] properties of HM. The micromechanical theory based on the Eshelby equivalence principle has been one important theoretical basis for determining structure–mechanical property relationships of HM, and has not only been employed to calculate elastic properties, but also developed to determine the thermoelastic and elastoplastic properties of HM.[9,10] These two important theoretical methods are often considered to be totally different from one another. In the present work, a simple correspondence relation between multiple-scattering and micromechanical theories will be suggested. The correspondence is of practical use in determining the structure–property relationships of HM within a unified theoretical framework.

Throughout this article, we use a general symbolic notation for the sake of convenience. All the tensors considered here are dyadic tensors, and the direct notation for tensors is used. This means that we ignore the subscripts to denote components of tensors. For example, stress tensor σ_{ij}, strain tensor ϵ_{ij}, and tensor of elastic moduli C_{ijkl}, are directly written as σ, ϵ, and C, respectively; and

$$C\epsilon = \sum_{k,l=l}^{3} C_{ijkl}\epsilon_{kl},$$

$$GC\epsilon = \sum_{k,l,m,n=1}^{3} G_{ijkl}C_{klmn}\epsilon_{mn} = \sum_{klmn} \int G_{ijkl}(x,x')C_{klmn}(x')\epsilon_{mn}(x')dx',$$

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and so on. These direct notations significantly simplify the resulting equations.

2 SCATTERING THEORY

Consider a perfectly bonded HM, its effective stiffness C^* being defined by

$$<\sigma>=C^*<\epsilon>, \quad (1)$$

where $<\sigma>$ and $<\epsilon>$ denote the average stress and strain tensor, respectively. The local stiffness C of the HM can be written as

$$C=C^{o}+C', \quad (2)$$

where C^{o} is the stiffness tensor of a homogeneous reference medium which can be arbitrarily selected, and C' is the fluctuation with respect to C^{o}. From the equilibrium equation, the following inhomogeneous differential equation can be obtained

$$C^{o}\nabla\cdot\epsilon+\nabla\cdot(C'\epsilon)=0 \quad (3)$$

An integral equation, which is equivalent to the equilibrium condition (3), can be written as

$$\epsilon=\epsilon^{o}+GC'\epsilon, \quad (4)$$

where ϵ^{o} is the homogeneous strain field under the surface displacement in the homogeneous reference medium, and G is the modified Green's function[3,4,8]

$$G_{ijkl}(x,x')=-\frac{1}{2}[g_{ik,jl'}(x,x')+g_{jk,il'}(x,x')], \quad (5)$$

where the commas in subscripts denote partial differentiation and the prime on l denotes the differentiation with respect to x'; Green's tensor $g_{ij}(x,x')$ satisfies the following equation and boundary conditions

$$C^{o}_{ijkl}g_{km,lj}(x,x')+\delta_{im}\delta(x-x')=0 \quad (6)$$

and

$$g_{ij}(x,x')\to 0,\ \text{as}\ |x-x'|\to\infty$$

The operator eqn (4) is satisfied by the iterative solution

$$\epsilon=\epsilon^{o}+GT\epsilon^{o}, \quad (7)$$

where T, called t-matrix tensor, is introduced

$$T=C'(I+GT)=C'(I-GC')^{-1}, \quad (8)$$

here I is the unit tensor. These equations lead to the effective stiffness[4]

$$C^*=C^{o}+<T><I+GT>^{-1}. \quad (9)$$

The problem now reduces to the task of computing $<T>$. Although eqn (9) is generally an exact result, the evaluation of $<T>$ is very difficult except for some simple cases.

The stiffness C^{o} of the homogeneous reference medium in eqn (9) can be arbitrarily-chosen. In approximate theories, there are two kinds of good choices. (1) $C^{o}=C_1$, i.e. the matrix phase (the first phase) of the HM under study is taken as the reference medium, which is a reasonable approach when the volume fraction of the included phase is very small. This approximation is known as the average t-matrix approximation (ATA);[3] (2) $C^{o}=C^*$, i.e. the constituent phases are embedded into a self-consistent effective medium with a yet unknown stiffness C^*. This approximation is called coherent potential approximation (CPA) or self-consistent effective medium approximation.[3]

Similarly, the thermoelastic problem of HM defined as

$$<\sigma>=C^*<\epsilon>-\beta^*\theta, \quad (10)$$

can be addressed. Here θ is a uniform temperature change; $\beta^*=C^*\alpha^*$, and α^* is the effective thermal expansion coefficient tensor. Equation (10) can be rewritten in the following more general form

$$<\sigma>=C^*(<\epsilon>-\epsilon^*),$$

where ϵ^* is a stress-free strain. Analogous to eqn (7), we can obtain

$$\epsilon=(I+GT)\epsilon^{o}-(I+GT)G\beta\theta. \quad (11)$$

As shown in Ref. 7, this leads to

$$\beta^*=<[I-(C^*-C^{o})G](I+TG)\beta>. \quad (12)$$

3 MICROMECHANICAL MODELS

Under given homogeneous surface displacement conditions, the local uniform strain within an inclusion is given by

$$\epsilon=A\epsilon, \quad (13)$$

where ϵ^{o} denotes the homogeneous strain in the homogeneous reference medium with the elastic moduli C°, and the fourth-order tensor A is called as the concentration factor and related to Eshelby's S-tensor[11]

$$A = [I + SC^{\circ -1}(C - C^{\circ})]^{-1}, \tag{14}$$

where the Eshelby's S-tensor can be found by using Green's function for the homogeneous medium.[5]

For the thermoelastic problem, eqn (13) can be rewritten as

$$\epsilon = A\epsilon^{0} - \mathbf{a}\theta, \tag{15}$$

where $\mathbf{a}$ is the thermal concentration factor which is a second-rank tensor. These equations also lead to the effective elastic properties of the HM[9]

$$C^{*} = C_1 + \left[\sum_i f_i(C_i - C_1) < A >_i\right] < A >^{-1}, \tag{16}$$

$$\beta^{*} = \beta_1 + \sum_i f_i A_i^{T}(\beta_i - \beta_1), \tag{17}$$

where $<\cdots>_i$ denotes averaging with respect to the ith phase, A_i^{T} is the transpose of A_i, f_i is the volume fraction of the ith phase. In any actual system, A and $\mathbf{a}$ are not known exactly. Instead, they are estimated by certain approximate procedures. The dilute approximation, the Mori–Tanaka methods,[12] and self-consistent method[11,13] are often employed for this purpose. In the dilute approximation and the Mori–Tanaka method, a matrix-based multiphase medium is considered as a collection of non-interacting inhomogeneties. In the self-consistent method each particle sees the effective medium of a yet unknown moduli.

4 THE CORRESPONDENCE RELATION

The effective thermoelastic properties, eqns (9) and (12), which are derived in multiple-scattering theory, appear to be different from the micromechanics results, eqns (16) and (17). They have often been considered as different theories. However, both theories start from a Green's function problem for the displacement field in a homogeneous medium. The multiple-scattering theory directly employs the Green's function solution, while the micromechanical theory indirectly employs the Green's function solution by the Eshelby's S-tensor. Therefore, both of them should correspond to each other, i.e. a connecting relationship can be anticipated.

By comparing eqns (7) and (13), and (11) and (15), we obtain directly

$$A = I + GT, \tag{18}$$

$$\mathbf{a} = (I + GT)G\beta. \tag{19}$$

Again by using (8) and (14), we can obtain

$$T = (C - C^{\circ})A, \tag{20}$$

$$G = -SC^{\circ -l}. \tag{21}$$

These equations constitute the simple correspondence relation between multiple-scattering theory and micromechanics models.

Alternatively, eqn (9) can be rewritten by the equivalent expression

$$C^{*} = C_1 + \left[\sum f_i(C_i - C_1) < [I - G - C^{\circ})]^{-1} >_i\right] \left\langle [I - G(C_1 - C^{\circ})]^{-1} \right\rangle^{-1}. \tag{22}$$

Comparison of (16) and (22) also gives the same relation

$$A = [I - G(C - C^{\circ})]^{-1} = I + GT. \tag{23}$$

For HM, the total t-matrix tensor can be rewritten as

$$T = \sum_n T_n + \sum_{n \neq m} T_n G T_m + \cdots, \tag{24}$$

where the first term is the sum of the t-matrix of n particles, and each of the successive terms represents the interactions of two-body, three-body, ..., among particles. This series is very difficult to calculate. To overcome this difficulty, the total t-matrix T is generally written as a first approximation, i.e.

$$T \cong \sum_n T_n = \sum_n C'_n(I - GC'_n)^{-1}, \tag{25}$$

which means many-body interactions among particles are ignored. This is the approximate multiple-scattering theory in practical applications.

In terms of the correspondence relation, we can rewrite ATA and CPA of the multiple-scattering theory by using micromechanical-based results. For simplicity, next we only discuss the elastic moduli. For ATA, we have

$$C^{*} = C_1 + \sum_i f_i(C_i - C_1)A_i\left[I + \sum_i f_i(A_i - I)\right]^{-1}. \tag{26}$$

This is just the Mori-Tanaka approximation.[12] Therefore, the ATA of the multiple-scattering theory corresponds to the Mori–Tanaka method of the micromechanical theory.

Similarly, the CPA can be expressed as

$$<T>=\sum_i f_i(C_i-C^*)A_i=0, \tag{27}$$

and this corresponds to the self-consistent method of the micromechanical theory. But the CPA is a symmetric self-consistent approximation in which each phase, including the matrix and the inclusion phases, is symmetrically treated; while the self-consistent method[13] of the micromechanical theory is an asymmetric one which asymmetrically treats the matrix and the inclusion phases like ATA. The CPA self-consistent condition, $<T>=0$, corresponds to a zero net polarization field, $<P>=0$, for electrical (and dielectric) problems. The self-consistent condition of the micromechnics-based method, $\sum f_iA_i=I$, corresponds to the self-consistency condition that the effective field is given by the algebraic average of the internal fields of each phase, $<E>=\sum f_iE_i$, for the electrical problem. These two self-consistency approximations yield the same results for a medium composed of spherical particles, but give different results for the case of ellipsoidal particles.[14] As the matrix and the inclusions have very different geometries, we prefer the self-consistent approximation of the micromechanics-based methods.

It is easy to show that the results estimated from (26) and (27) by using the concentration factors of the micromechanics-based theory are identical to those directly obtained from (9) by approximate multiple-scattering theories. For simplicity, consider a general isotropic composite composed of spherical particles. In this case, we can obtain the ATA for effective bulk modulus k^* and the effective shear modulus m^* of the composite from (26)

$$\begin{aligned}\frac{k^*-k_1}{3k^*+4\mu_1}&=\sum_{i=2}f_i\,\frac{k_i-k_1}{3k_i+4\mu_1},\\ \frac{\mu^*-\mu_1}{\mu^*+y_1}&=\sum_{i=2}f_i\,\frac{\mu_i-\mu_1}{\mu_i+y_1}\end{aligned} \tag{28}$$

where

$$y_1=\frac{\mu_1(9k_1+8\mu_1)}{6k_1+12\mu_1},$$

These results are exactly those obtained directly by computing $<T>$ from (9),[14] and also identical to micromechanical results.[12,15] Similarly, the CPA solution can be obtained from (27)

$$\begin{aligned}\sum_{i=1}f_i\,\frac{ki-k^*}{3k_i+4\mu^*}&=0,\\ \sum_{i=1}f_i\,\frac{\mu_i-\mu^*}{\mu_i+y^*}&=0,\end{aligned} \tag{29}$$

where $y^*=y(k^*,\mu^*)$, eqn (28c). These results are also precisely those obtained directly by computing $<T>$.[14] In the case of the spherical constituent particles, the CPA results (29) coincide with the self-consistent results of the micromechanical model.[11,13] In the case of spheroidal particles, such as needle and disk shaped particles, the CPA gives symmetrically self-consistent results[14] which are different from the asymmetrically self-consistent results[13] of the micromechanical model. The discussion above also applies to the effective thermal strains.

5 CONCLUSIONS

In this work, a relation between the multiple-scattering theory and micromechanical models of effective materials properties of HM has been established. Two approximations, ATA and CPA, of the multiple-scattering theory are found to be correspondent to the Mori–Tanaka and self-consistent approximations of the micromechanical models, respectively. The ATA and CPA are then given in terms of the micromechanics-based results. The combination of these two theories gives three approximations, i.e. ATA (or Mori–Tanaka approximation), symmetric self-consistency approximation (CPA), and asymmetric self-consistency approximation. As a final remark, we want to emphasize that the ATA and CPA discussed above are only first-order approximations of the multiple-scattering theory. The second (or higher) -order approximations containing microstructural information, such as the spatial distribution of particles and interactions, can be in principle obtained by computing the second term of the total t-matrix tensor (24). However, the microstructural information cannot be directly incorporated into micromechanical models.

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