A micromechanical method for particulate composites with finite particle concentration

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Abstract

Many micromechanical models can be obtained by embedding one single ellipsoidal pattern into matrix material to derive localization relation, the direct influence of the other patterns is neglected. An extension of Ponte Castaneda and Willis model (PCW) [J. Mech. Phys. Solids 43 (1995) 1919] to many patterns interaction is proposed for particulate composites with an ellipsoidal distribution of particles. Compared to the models based on one single spherical pattern (Mori–Tanaka model [Acta Metall. 21 (1973) 571] for an isotropic composite) or based on one single ellipsoidal pattern (PCW model for an transverse isotropic composite due to ellipsoidal distribution of particles), the proposed method gives better prediction on the overall elastic properties for particulate composites with finite particle concentration. The extension of the elastic results directly to plasticity are performed with the help of secant moduli method based on second-order stress moment, the prediction on the overall elastic and plastic properties for particulate composites agrees well with the experimental results in literature.

Keywords: Micromechanics; Particulate composites; Plasticity; Finite particle concentration; Anisotropy

1. Introduction

Objective of micromechanics is to bridge the macroscopic property of heterogeneous materials from their microstructural parameters. To this end, a number of models have been proposed, for example Mori and Tanaka (1973) model, self-consistent method (Hershey, 1954), generalized self-consistent model (Christensen and Lo, 1979), and some more recently proposed models such as double inclusion model (Hori and Nemat-Nasser, 1993), Ponte Castaneda–Willis model (Ponte Castaneda and Willis, 1995) and effective self-consistent method (Zheng and Du, 2001). With the concept of pattern introduced by Bornert et al. (1996), Hu and Weng (2000a), and Hu et al. (2001) have shown that, in above-mentioned methods, the localization relation is determined by embedding one single isolate pattern into a reference material. The pattern is usually chosen to be a double ellipsoidal type: an ellipsoidal inhomogeneity is surrounded by another ellipsoidal cell. The outer ellipsoidal cell is used to characterize local inhomogeneity distribution (Ponte Castaneda and
Willis, 1995; Hu and Weng, 2000a,b; Hu et al., 2001; Zheng and Du, 2001). By choosing the reference material to be the yet unknown composite, this leads to generalized self-consistent estimation, and if the matrix is taken for the reference material, the Mori–Tanaka method, double inclusion model, Ponte Castaneda–Willis model, and effective self-consistent method can be recovered by judiciously choosing the orientation and shape of the double cells (Hu and Weng, 2000a; Hu and Weng, 2000b; Hu et al., 2001). This means that the previous methods (apart from self-consistent and generalized self-consistent method) are intrinsically dilute in the sense that only one isolated pattern is placed into the matrix material for deriving the localization relation, the direct influence of the other patterns is ignored. Their predictions may deviate from experimental results if the volume concentration of particles becomes large, as shown by Ju and Chen (1994) for the Mori and Tanaka (1973) model, a particular case of PCW method for the isotropic distribution of particles. The objective of this paper is to generalize these models for finite particle concentration by considering many pattern interaction while conserving their beautiful structures.

As concern as the modeling for finite concentration of particles, Ju and Chen (1994) proposed an interesting model for isotropic composites by considering the statistical interaction of two spherical particles. Molinari and Mouden (1996) proposed to solve approximately a multi-particles problem and they obtained the corresponding localization relation. Another route for the finite concentration modeling is to introduce a high order correlation function up to the third-order, as the third-order bounds proposed by Beran and Molyneux (1966); Milton (1981) and summarized by Toquato (1991). An third-order estimate for the shear and bulk moduli for an isotropic composite is recently proposed by Torquato (1997, 1998), which indeed improves the estimation for a finite concentration of particles.

In this paper, we will propose an analytical micromechanical model for predicting the elastoplastic behavior of an anisotropic composite with finite particle concentration, and the ellipsoidal distribution of particles introduced by Ponte Castaneda and Willis (1995) is conserved for modeling the overall anisotropic behavior of composites. The paper will be arranged as follows: the theoretical formulation of the problem is presented in Section 2, including the main idea, a new way to determine localization relation, and also the method to extend the elastic results directly to plasticity; extensive numerical examples concerning the overall modulus and the effective elastoplastic stress–strain relations of isotropic and transversely isotropic composites are presented in Section 3; the conclusion will be given in Section 4.

2. Formulation of problem

2.1. Effective elastic properties of composites

In this paper, we will consider particulate composite with an ellipsoidal distribution of particles, proposed by Ponte Castaneda and Willis (1995). As discussed in the introduction, many micromechanical models simplify the multi-pattern interaction problem by considering only one single pattern in a reference material. When the reference material is taken to be the matrix material, this leads to the Ponte Castaneda–Willis estimate, and for the isotropic distribution of the particle, the Mori–Tanaka’s method is derived. As well know that Mori–Tanaka’s method cannot give good prediction for large particle concentration, this is, according to our opinion, due to the fact that only one pattern is considered to build the localization relation. In this paper, a new model will be proposed to consider the direct interaction of the particle. The main idea of this work consists of generalization of Ponte Castaneda–Willis model for considering multi-particle interactions. Fig. 1(a) and (b) show respectively the problems solved for the localization relation by Ponte Castaneda–Willis model and by the proposed method.

In PCW model, a single pattern of one particle enclosed by an ellipsoidal cell is placed into the matrix material under a reference strain. The volume of particles to that of the outer ellipsoidal cell is the particle volume fraction of the composite, the detailed discussion of PCW method can be found in references (Hu and Weng, 2000a,b
In the present model, we choose a large ellipsoid having the same shape and orientation of the outer ellipsoidal cell of the pattern, in this large ellipsoid many single patterns are included to consider the direct interaction of the particles, and this large pattern is placed into the matrix material. When the outer cell of the pattern is of a spherical shape, PCW model in this case reduces to Mori–Tanaka’s estimate, and the proposed method will give the estimation of an isotropic composite with finite particle concentration.

In the following, the problem to be solved with infinite number of the particles with varying size is simplified by finite number of mono-size particles, as illustrated in Fig. 2. For an ellipsoidal distribution, the ratio of average distance of particles in the major axis direction of the distribution ellipsoid to that in the minor axis direction is set to equal to the aspect ratio of the distribution ellipsoid, this is shown in Fig. 2, and the total volume fraction of particles to that of the distribution ellipsoid is the volume fraction of particles for the actual composite.

Assuming that there are \( N \) particles in the ellipsoidal region, if we can determine the average stresses in these particles, and note them by

\[
\varepsilon_i = \mathbf{H}_i : \mathbf{E}^0
\]

where the index \( i \) ranges from 1 to \( N \).

From an elementary micromechanical analysis, the following exact relation holds (Hu and Weng, 2000a)

\[
(\mathbf{L}_c - \mathbf{L}_0) : \mathbf{E} = \sum_{i=1}^{N} c_i (\mathbf{L}_i - \mathbf{L}_0) : \varepsilon_i
\]

where \( \mathbf{L}_c, \mathbf{L}_0 \) and \( \mathbf{L}_i \) are the modulus tensors for the composite, matrix and \( i \)th particle respectively. \( c_i \) is volume fraction of the \( i \)th particle. There is no summation for the repeated indices.

With help of Eqs. (1) and (2) and noting that there is only one population of particles, we have
\[(L_c - L_0) : E = f(L_1 - L_0) \mathbf{H} : E^0\]  \tag{3}

where \(\mathbf{H} = \frac{1}{N} \sum_{i=1}^{N} \mathbf{H}_i\), \(f\) is the volume fraction of the particle for the composite. In order to eliminate the reference strain \(E^0\) by the composite strain \(E\), here in this paper we will make use of the concept introduced by Kuster and Toksöz (1974), which is shown to be equivalent to the Ponte Castaneda–Willis model (Hu and Weng, 2000a).

Now place an ellipsoid of the composite material into a reference material (here the reference material is the matrix) under the same remote strain \(E^0\) (Fig. 3), the shape and orientation of the composite ellipsoid are the same as those of the ellipsoid characterizing the distribution of the particle. From the Eshelby’s inclusion theory (Eshelby, 1957), we get the strain in the composite \(E\) as

\[E = G_c : E^0\]  \tag{4}

where \(G_c = (L_0 - L_c)^{-1} : L_0 : A_c\), \(A_c = -[S^0 - (L_0 - L_c)^{-1} : L_0]^{-1}\) and \(S^0\) is the Eshelby tensor for the composite inclusion.

From Eqs. (3) and (4), the effective modulus tensor of the composite can then be derived as

\[L_c = L_0 : \left\{I - f[(I - M_0 : L_1) : \mathbf{H}]^{-1} + fS^0]^{-1}\right\}\]  \tag{5}

where \(M_0\) is the compliance tensor of the matrix.

Now the problem is focused on evaluation of the quantity \(\mathbf{H}\), numerical methods can be employed (Shen et al., submitted), however in this paper an approximate analytical method will be proposed.

Now consider an infinite matrix containing randomly located \(N\) particles, a remote strain \(E^0\) is applied. According to the method proposed by Zeller and Dederichs (1973), the strain at any location \(r\) can be expressed by

\[\varepsilon(r) = E^0 - \sum_{i=1}^{N} \gamma_i(r - r') : \left[(L_1 - L_0) : \varepsilon_i(r')\right] \, dr'\]  \tag{6}

where \(\gamma_i(r - r')\) is the modified Green function, \(V_i\) is the region occupied by the \(i\)th particle.

Averaging Eq. (6) over the particle \(j\) \((j = 1, 2, \ldots, N)\), then

\[\bar{\varepsilon}_j = E^0 - \sum_{i=1}^{N} \frac{1}{V_j} \int_{V_j} \int_{V_j} \gamma_i(r - r') : \left[(L_1 - L_0) : \varepsilon_i(r')\right] \, dr' \, dr\]  \tag{7}

where \(\bar{\varepsilon}_j\) is average strain in the \(j\)th particle.

In order to proceed, here we assume that the strain in the particle \(i\) \((i = 1, 2, \ldots, N)\) is uniform, but it is different for different particles, then Eq. (7) becomes

\[\bar{\varepsilon}_j = E^0 - \sum_{i=1}^{N} B^{ij} : \bar{\varepsilon}_i\]  \tag{8}

where \(B^{ij} = \frac{1}{V_j} \int_{V_j} \int_{V_i} \gamma_i(r - r') \, dr' \, dr\) : \((L_1 - L_0)\), when \(i = j\), \(B^{ij}\) are the Eshelby tensor for a spherical inclusion, and \(i \neq j\), \(B^{ij}\) characterizes the interaction between the particle pair \(i\) and \(j\). The analytical expressions are derived by Berveiller and Fassi-Fehri (1987), they are listed in the Appendix A after a minor correction of printed errors.

Expression (8) provides \(N\) equations to determine \(\mathbf{H}_i\), in turn \(\mathbf{H}\), and the effective modulus tensor of the composite with finite concentration of particles can then be evaluated from Eq. (5). It is clear that when the particle volume fraction is small, the direct influence of the patterns can be neglected, the localization problem can be deter-
determined by only one single ellipsoidal pattern, the proposed method reduces in this case to Ponte Castaneda–Willis model.

2.2. Elastoplastic behavior of composites with finite particle concentration

It is of interest to examine also the effective nonlinear property of composites with the proposed method. Here we will use the secant moduli method based on second-order stress moment developed by Qiu and Weng (1992), and Hu (1996). This method, apparently simple, has a firm theoretical basis, it can be interpreted as the variational method proposed by Ponte Castaneda (1991), as demonstrated by Suquet (1995) and Hu (1996).

Assuming that the matrix material follows a power type hardening law

\[ \sigma_s = \sigma_{y0} + h (\varepsilon_p)^n \]  

(9)

where \( \sigma_{y0} \), \( h \) and \( n \) are initial yield stress, strength coefficient, and work-hardening exponent respectively, and \( \varepsilon_p \) is effective plastic strain.

The secant shear and bulk moduli of the matrix at plastic strain \( \varepsilon^p \) are defined as

\[ \mu^s = 1/(1/\mu_0 + 3\varepsilon^p / (\sigma_{y0} + h (\varepsilon^p)^n)), \quad k^s = k_0 \]  

(10)

where \( k_0 \) and \( \mu_0 \) are the elastic bulk and shear moduli of the matrix.

The idea of the secant moduli method can be explained as follows: for any applied \( \Sigma \) the matrix is in plastic state, if the effective plastic strain of the matrix \( \varepsilon^p \) is known, then the secant moduli of the matrix (Eq. (10)), the composite secant moduli is set to be the elastic moduli of a linear comparison composite, this linear comparison composite has the same microstructure as the actual composite, and the elastic modulus of the matrix for the linear comparison composite is set to the secant modulus of the actual matrix. In order to determine the evolution of the effective plastic strain of the matrix \( \varepsilon^p \) as function of the applied load \( \Sigma \), we have to evaluate the average effective stress in the matrix for the linear comparison composite, this can be done with the method proposed by Hu (1996),

\[ \sigma^2_s = 3/2(\mathbf{s} : \mathbf{s})_0 = \Sigma : \left[ -\frac{3\mu^0}{1-f} \frac{\partial \mathbf{M}^c}{\partial \mu^0} \right] : \Sigma \]  

(11)

where \( \mathbf{M}^c \) is the secant compliance tensor of the actual composite or the elastic compliance tensor of the linear comparison composite, and it can be determined with the proposed method in Section 2.1 (Eq. (5)). \( (\mathbf{c})_0 \) denotes the average of the said quantity over the matrix, \( s \) is the deviatoric part of a stress tensor.

With the proposed method for the effective moduli and the secant moduli method for plasticity, the elastoplastic behavior of a particulate composite can then be determined for an ellipsoidal distribution and finite concentration of particles. In the following section, the predicted capacity of the proposed method will be illustrated through some numerical examples and it will also be compared with available experimental results.

3. Numerical application

3.1. Isotropic composite

For an isotropic composite, the ellipsoid for the particle distribution becomes a sphere, and the Mori–Tanaka’s method corresponds to the case of one single spherical pattern. We also compare the predicted results with the method proposed by Ju and Chen (1994), the third-order estimate by Torquato (1997), and also the experimental measurement conducted by Simth (1976). The Young’s modulus and Poisson’s ratio of the matrix and particles are respectively \( E_0 = 3.0 \) GPa, \( v_0 = 0.4 \), \( E_1 = 76 \) GPa and \( v_1 = 0.23 \); these data are taken from the work of Simth (1976).

In our computation, 27 particles are randomly placed in a spherical domain, it was also checked that 8 particles (the volume fraction is kept the same) suffice to give an accurate prediction. The comparison results on the effective Young’s modulus and effective shear modulus of the composite are shown respectively in Fig. 4(a) and (b).

For a particulate composite, it is found that the prediction by the present method correlates better with the experiment conducted by Simth (1976) than those of the Mori–Tanaka’s method and the third-order estimate, it gives almost the same results as that predicted by the method of Ju and Chen (1994). It is also seen that the Mori–Tanaka’s
method, a widely used model, underestimates severely the effective moduli for particle concentrations larger than 30% and the third-order estimate indeed improve the estimation compared to the lower bound estimate (Mori–Tanaka’s method), but it still underestimates the effective moduli for a relatively large volume concentration of particles (the particle is the harder phase). As expected, the proposed method converges to the Mori–Tanaka’s model for small particle concentrations.

Now we apply the proposed method for a porous glass, the experimental results are reported by Walsh et al. (1965). The matrix elastic constants are $E_0 = 75$ GPa and $v_0 = 0.23$, as also given by Walsh et al. (1965). The comparison results are shown in Fig. 5(a) and (b).

It is found that the proposed method again agrees well with the experimental data, this time the proposed method predicted a little stiffer bulk modulus than that given by Ju and Chen (1994), and the predictions for the effective shear modulus for the porous material are almost the same for the proposed method, Ju and Chen’s model and the third-order estimate.
As concern as the prediction of overall elasto-plastic property for composite materials, we apply the proposed method to a metal matrix composite, the experimental results are given by Yang and Picard (1991). The comparison results are shown in Fig. 6(a), the simulation of the matrix stress and strain curve is also included in the figure. For comparison, we also include the predicted results by Mori–Tanaka’s method in Fig. 6(b).

As shown in Fig. 6, the present method give a good prediction up to 50% particle volume fraction. On the contrary, Mori–Tanaka’s method gives a poor prediction even for 30% particle volume fraction. As demonstrated for elasticity and plasticity, the proposed method can be applied for predicting the elastoplastic behavior of isotropic composites with a high volume concentration of particles.

3.2. Anisotropic composite

The proposed method is very flexible, and it can be applied to predict the anisotropic behavior of composites for finite particle concentration due to an ellipsoidal distribution of particles. For small particle concentrations, the proposed method will reduce to PCW’s model or Kuster and Toksoz model, which is based on single ellipsoidal pattern for localization relation.

For an ellipsoidal distribution, to simplify the analysis, we firstly divide the distribution ellipsoid into different sites according to the condition described in Section 2.1, and then place the particles on these sites. As for the isotropic case, 27 particles are used in the computation, we have checked that 8 particles can also give an accurate prediction.

Since even for a spherical particle reinforced composite, due to the ellipsoidal distribution of particles, the composite as a whole is transversely isotropic (Fig. 7), it has five independent elastic constants. The aspect ratio of the distribution spheroid is set to be two in the computation. The predicted effective elastic constants by the present method are compared with those predicted by PCW’s method, which is the single pattern of the present method.

As shown in Fig. 8, compared to PCW’s method, as expected, the present method predicts stiffer responses for both shear and Young’s moduli in transverse and longitudinal directions respectively. The difference between the predicted results by the present and PCW’s models increases significantly with increase of particle volume concentration. It is also found that the difference in the transverse and longitudinal effective moduli of the composite is more pronounced by the present method.

With the secant moduli method based on second-order stress moment, the overall anisotropic plasticity of particulate composites can be easily
investigated. We take the same example as in the isotropic case for the material constants, the volume fraction of the hard particle is 26%. Fig. 9 shows the stress–strain curves predicted by the present method in the transverse and longitudinal direction respectively, they are also compared with the results predicted by PCW’s method. As for the isotropic case, the present method predicts significant stiffer responses compared to those by PCW’s method. For example for the composite at 0.6% macroscopic strain, the present method predicts the macroscopic stress about 250 MPa, and only 200 MPa by PCW’s method.

Fig. 9 overall stress–strain curves in transverse and longitudinal directions predicted by present method and PCW’s model ($f = 26\%$, aspect ratio of the distribution ellipsoid is 2).

Finally, it must emphasize that for an ellipsoidal distribution of particles, in order to realize this distribution, the aspect ratio of the distribution ellipsoid and the volume fraction of particles must satisfy some constraint conditions, as explained in

Fig. 7. Distribution of particles: (a) isotropic distribution; (b) ellipsoidal distribution.

Fig. 8. Comparison of present model and PCW’s model: (a) effective shear modulus; (b) effective Young’s modulus.

Fig. 9. Overall stress–strain curves in transverse and longitudinal directions predicted by present method and PCW’s model ($f = 26\%$, aspect ratio of the distribution ellipsoid is 2).
references (Ponte Castaneda and Willis, 1995; Hu and Weng, 2000b).

4. Conclusions

An analytical micromechanical method is proposed to predict the overall elastic and plastic properties of particulate composites with finite particle concentrations, this method generalizes one single pattern problem to many patterns interaction for deriving the localization relation, and it can take into account the particle interaction more accurately in case of finite concentration of particles. For an isotropic composite, the proposed method based on multi-patterns interaction gives better predictions compared to Mori–Tanaka’s method (based on one single spherical pattern), and for an anisotropic composite with an ellipsoidal particle distribution, the present method gives more stiffer predictions on overall moduli and elastoplastic stress and strain curves, compared to PCW’s method (one single ellipsoidal pattern). As expected, when volume concentration of particles is small, the proposed method of multiple ellipsoidal patterns reduces to PCW’s model.

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Appendix A. Expression fourth-order tensor $B^{rs}_{ijmn}$

For two spherical particles $r$ and $s$, $V_r$ and $x^r_i$ denote respectively the volume and position (the coordinate in the $i$th direction) of the particle $s$. We denote the distance of two particles by $\rho$, $n_i = (x^r_i - x^s_i)/\rho$, and $a, b$ are the radius of the particles $r$ and $s$ respectively. $\mu$ and $\nu$ are the matrix shear and Poisson ratio. The fourth-order tensor $B^{rs}_{ijmn}$ are given by (Mura, 1987).

\[
B^{rs}_{ijmn} = \frac{1}{16\pi\mu(1 - \nu)} \psi^{rs}_{ijmn} - \frac{1}{8\pi\mu} [\delta_{im}\psi^{rs}_{jn} + \delta_{jm}\psi^{rs}_{in}]
\]  

(A.1)

where

\[
\psi^{rs}_{ijmn} = -V_s \left( \frac{1}{\rho^3} \left( 1 - \frac{3}{5}k^2 \right) (\delta_{ij}\delta_{mn} + \delta_{im}\delta_{jn}
\right.
\]

\[
+ \frac{15}{\rho^5} \left( 1 - \frac{7}{5}k^2 \right) n_in_jn_mn_n
\]

\[
- \frac{3}{\rho^5} (1 - k^2)(\delta_{ij}n_mn_n + \delta_{im}n_jn_m + \delta_{jm}n_in_n
\]

\[
+ \delta_{in}n_jn_m + \delta_{jn}n_in_m + \delta_{mn}n_in_j) \right)
\]

(A.2)

\[
\phi^{rs}_{ij} = -V_s \left( \frac{\delta_{ij} - 3n_in_j}{\rho^5} \right)
\]

(A.3)

and

\[
k^2 = \frac{a^2 + b^2}{\rho^2}
\]

(A.4)

From above equations, we get, if the two particles are placed along $Ox_3$, the expressions for the components of $B^{rs}_{ijmn}$ for $r \neq s$, which were given for the first time by Berveiller and Fassi-Fehri (1987)

\[
B^{rs}_{1111} = B^{rs}_{2222} = \frac{V_s}{16\pi\rho^3} \frac{1}{\mu(1 - \nu)} \left( 1 - 4\nu + 9\frac{k^2}{5} \right)
\]

\[
B^{rs}_{1112} = B^{rs}_{2211} = \frac{V_s}{16\pi\rho^3} \frac{1}{\mu(1 - \nu)} \left( 1 + 3\frac{k^2}{5} \right)
\]

\[
B^{rs}_{1133} = B^{rs}_{2233} = B^{rs}_{3311} = B^{rs}_{3322} = \frac{V_s}{16\pi\rho^3} \frac{1}{\mu(1 - \nu)} \left( 2 - 12\frac{k^2}{5} \right)
\]

\[
B^{rs}_{1212} = B^{rs}_{1221} = B^{rs}_{2112} = B^{rs}_{2121} = \frac{V_s}{16\pi\rho^3} \frac{1}{\mu(1 - \nu)} \left( 1 - 2\nu + 3\frac{k^2}{5} \right)
\]

\[
B^{rs}_{1313} = B^{rs}_{3131} = B^{rs}_{3113} = B^{rs}_{3313} = \frac{V_s}{16\pi\rho^3} \frac{1}{\mu(1 - \nu)} \left( 1 + \nu - 12\frac{k^2}{5} \right)
\]

\[
B^{rs}_{2323} = B^{rs}_{3232} = B^{rs}_{3223} = \frac{V_s}{16\pi\rho^3} \frac{1}{\mu(1 - \nu)} \left( 1 + \nu - 12\frac{k^2}{5} \right)
\]

\[
B^{rs}_{3333} = \frac{V_s}{16\pi\rho^3} \frac{1}{\mu(1 - \nu)} \left( -8 + 8\nu + 24\frac{k^2}{5} \right)
\]
If \( r = s \), \( B_{ijmn}^{rs} \) is degenerated to \( S_{ijkl} M_{klmn} \), where \( S_{ijkl} \) is the Eshelby tensor for a spherical inclusion, \( M_{klmn} \) is compliance tensor of the matrix material.

References


