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Some reflections on the Mori-Tanaka and Ponte Castañeda-Willis methods with randomly oriented ellipsoidal inclusions

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Summary. For a two-phase isotropic composite consisting of an isotropic matrix and randomly oriented isotropic ellipsoidal inclusions, Mori-Tanaka's (MT) [6] method and the more recent Ponte Castañeda-Willis (PCW) [1] method are perhaps the only two methods that deliver explicit results for its effective moduli. An attractive feature of the MT method is that it always stays within the Hashin-Shtrikman [3] bounds, while the novel part of the PCW approach is that it has a well defined microstructure. In this paper, we made a comparative study on these two models, for both elasticity and their applications to plasticity. Over the entire range of inclusion shapes, the PCW estimates are found to be consistently stiffer than the MT estimates. An investigation of the possibility of a PCW microstructure for the MT model indicates that the MT moduli could be found from the PCW formulation, but this would require a spatial distribution that is identical to the oriented inclusion shape. Such a requirement implies that the underlying two-point joint probability density function is not symmetric, and thus it is not permissible. One is led to conclude that, unlike the aligned case, the MT model cannot be realized from the PCW microstructure with randomly oriented inclusions.

1 Introduction

In a recent paper Ponte Castañeda and Willis (PCW) [1] proposed a method to estimate the effective elastic moduli of a two-phase composite whose microgeometry can be described by some statistical distribution functions. A novel feature of this method is that the spatial distribution of inclusions can be separated from the inclusion shape, and the results are explicit. The development was based on the Hashin-Shtrikman (HS) [2], [3] variational structure put forward by Willis [4], [5]. While there exist several other promising micromechanical models – such as the composite sphere and cylinder assemblages, and the generalized self-consistent scheme – they are somewhat limited in terms of the inclusion shape. The self-consistent and the differential schemes are both capable of accounting for the effect of inclusion shape, but the results are implicit.

The only other micromechanical model which is also explicit, and can account for various inclusion shapes and orientations, is perhaps Mori and Tanaka's (MT) [6] method. This method was originally developed with the simple assumption that the perturbed strain in the inclusions – even at a non-dilute concentration – is connected to the eigenstrain through Eshelby's [7] S-tensor of a single inclusion problem. As such, the model was not developed from consideration of microgeometry, and is in principle reliable only when the inclusion concentration is not high. But it turns out that, with spherical inclusions, the MT moduli always coincide with the HS lower (or upper) bounds when the matrix is the softer (or harder) phase

[8], and that with randomly oriented spheroidal inclusions the effective moduli also always stay within the HS bounds as the shape of the inclusions changes from sphere to flat disk [9]. With two isotropic phases, the MT moduli never violate the bounds even at high concentration. Several of its basic properties are also consistent with Walpole's [10], [11] theory for anisotropic phases [12]. Moreover, with aligned ellipsoidal inclusions, it is now known to possess the Willis [4] microgeometry in which the inclusion distribution and the inclusion shape are jointly accounted for by the same ellipsoidal function [1], [13].

While the microgeometrical affiliation of the MT model in the aligned case is now understood, its position in the randomly oriented case remains unclear, apart from the fact that it never violates the HS bounds. The availability of the PCW microstructure with randomly oriented inclusions now permits one to examine the MT estimates one step further, at least to the extent whether the MT estimates are higher or lower than the PCW estimates. The explicit nature of both models also renders themselves particularly suitable for applications to the elastoplastic behavior of a composite through a scheme recently developed by Ponte Castañeda [14], Suquet [15], Tandon and Weng [16], and Qiu and Weng [17] in conjunction with Hu [18]. This will be the second focus of this study. At the end some observations will be made on whether the MT model has a realizable microstructure from PCW's formulation.

2 General formulae of the PCW and MT methods

To put the present study in proper perspective it is useful to recall the PCW theory first. More complete account should of course go to the original work. The MT method has been recited by Weng [8], [12], and Benveniste [19], among others, and thus it will not be repeated here.

Let the moduli tensors of the matrix and inclusions be denoted by L_0 and $L_r\,(r = 1, \dots N)$, respectively, and the inclusions are taken to be ellipsoidal in shape. A uniform macroscopic strain tensor $\bar{\boldsymbol{\varepsilon}}$ is prescribed on the representative volume element of the composite. The distribution of the inclusion is also taken to possess an ellipsoidal symmetry; that is, the conditional probability density function $p^{r|s}(z'')$ can be written as $p^{r|s}(z'') = \phi_{rs}(Z_d{}^{rs} : z'')$, which represents the probability density for finding an inclusion r centered at z given that there is an inclusion s centered at z', with $z'' = z - z'$. The matrix $Z_d{}^{rs}$ defines an ellipsoid $\Omega_d{}^{rs} = \{x : |Z_d{}^{rs} : x|^2 < 1\}$ for each inclusion, serving to characterize the distribution of inclusions. Inside the ellipsoid $\Omega_d{}^{rs}, p^{r|s} = 0$. The estimates or bounds for the effective moduli tensor of the composite then can be written as

$$L_{PCW} = L_0 + L\,, \tag{1}$$

where L is determined by $\tau = \sum_{r=1}^{N} c_r \tau^r = L : \bar{\boldsymbol{\varepsilon}}$, and c_r is the volume concentration of inclusions of type r. The piecewise uniform polarization stress τ^r in the phase or orientation r satisfies

$$[(L_r - L_0)^{-1} + P_i^r]\,\tau^r - \sum_{s=1}^{N} c_s P_d{}^{rs} : \tau^s = \bar{\boldsymbol{\varepsilon}}\,, \tag{2}$$

where $P_i^r = \int_{\Omega^r} \Gamma^0(x - x')\,dx'$ with $x \in \Omega^r$, and $P_d{}^{rs} = \int_{\Omega_d{}^{rs}} \Gamma^0(x - x')\,dx'$ with $x \in \Omega_d{}^{rs}$. In addition $\Gamma^0(x - x')$ is the modified Green's function for the infinite medium with a stiffness tensor L_0, and Ω^r is the region occupied by the inclusion of type r. From the definition of conditional probability one has $P_d{}^{rs} = P_d{}^{sr}$.

When the distribution of the inclusions is taken to be the same for all inclusion pairs (i.e., ${\Omega_d}^{rs} = \Omega_d$, or ${P_d}^{rs} = P_d$ for all $r, s = 1, \ldots N$), the effective moduli tensor can be written simply as

$$L_{PCW} = L_0 + \left[I - \sum_{r=1}^{N} c_r T_r P_d\right]^{-1} \left[\sum_{r=1}^{N} c_r T_r\right], \tag{3}$$

where $T_r = [(L_r - L_0)^{-1} + P_i^r]^{-1}$, and I is the fourth-order identity tensor.

For comparison, Mori-Tanaka's moduli can also be cast into [8], [12], [20]

$$L_{MT} = L_0\left[I + \sum_{r=1}^{N} c_r Q_r \cdot \left(I - \sum_{r=1}^{N} c_r S_r Q_r\right)^{-1}\right], \tag{4}$$

where

$$Q_r = [(L_r - L_0)\, S_r + L_0]^{-1}\, (L_r - L_0)\,, \tag{5}$$

and S_r is Eshelby's tensor for the inclusion of type r.

3 A two-phase isotropic composite containing randomly oriented isotropic ellipsoidal inclusions

We now focus on the declared problem: a two-phase composite consisting of an isotropic matrix and randomly oriented isotropic ellipsoidal inclusions. The foregoing summation process then can be replaced by the orientational average $< . >$, and the PCW moduli can be rewritten as

$$L_{PCW} = L_0 + c_1[I - c_1 < T > P_d]^{-1} < T >, \tag{6}$$

where c_1 is the volume concentration of phase 1 (inclusions) and the subscript r in T has been dropped for brevity. The values of P_i and P_d are related to Eshelby's S through as $P_i = S{L_0}^{-1}$ and $P_d = S_d {L_0}^{-1}$ in the local oriented axes, with S and S_d further related to the aspect ratios w and w_d of the ellipsoids Ω and Ω_d, respectively (the subscript d will continue to be carried to designate the spatial distribution).

With the additional relation $T = L_0 Q$, the PCW moduli can be recast into

$$L_{PCW} = L_0\{I + c_1[< Q >^{-1} - c_1 S_d]^{-1}\}\,. \tag{7}$$

On the other hand, the MT moduli can also be evaluated with the orientational average as

$$L_{MT} = L_0[I + c_1(< Q >^{-1} - c_1 < SQ >< Q >^{-1})^{-1}]\,. \tag{8}$$

Then with the help of the identities

$$QS = I - Q(L_1 - L_0)^{-1}\, L_0\,, \qquad SQ = I - (L_1 - L_0)^{-1}\, L_0 Q \tag{9}$$

it leads to

$$L_{MT} = L_0\{I + c_1[(1 - c_1) < Q >^{-1} + c_1(L_1 - L_0)^{-1}\, L_0]^{-1}\}\,. \tag{10}$$

At this stage it is instructive to cast the PCW and MT moduli – (7) and (10), respectively – in terms of the bulk and shear components. When the distribution of the ellipsoids is taken to be spherically symmetric as considered in [1], one has

$$S_d = (\alpha_0, \beta_0), \qquad \text{with} \quad \alpha_0 = \frac{1}{3}\frac{1+\nu_0}{1-\nu_0}, \qquad \beta_0 = \frac{2}{15}\frac{4-5\nu_0}{1-\nu_0}, \tag{11}$$

where ν_0 is Poisson's ratio of the matrix. Furthermore, in terms of the bulk and shear moduli of the phases, one has $L_0 = (3\varkappa_0, 2\mu_0)$, $L_1 = (3\varkappa_1, 2\mu_1)$, and $(L_0^{-1}L_1 - I)^{-1} = [\varkappa_0/(\varkappa_1 - \varkappa_0), \mu_0/(\mu_1 - \mu_0)]$. The orientational average of $< Q >^{-1}$ can also be cast in an isotropic form,

$$< Q >^{-1} = (Q_\alpha, Q_\beta), \tag{12}$$

so that

$$\frac{\varkappa_{PCW}}{\varkappa_0} = 1 + \frac{c_1}{Q_\alpha - c_1\alpha_0}, \qquad \frac{\mu_{PCW}}{\mu_0} = 1 + \frac{c_1}{Q_\beta - c_1\beta_0}, \tag{13}$$

and

$$\frac{\varkappa_{MT}}{\varkappa_0} = 1 + \frac{c_1}{(1-c_1)\,Q_\alpha + c_1\varkappa_0/(\varkappa_1 - \varkappa_0)}, \qquad \frac{\mu_{MT}}{\mu_0} = 1 + \frac{c_1}{(1-c_1)\,Q_\beta + c_1\mu_0/(\mu_1 - \mu_0)}. \tag{14}$$

Evaluation of $< Q >^{-1}$ leads to

$$Q_\alpha = a + 3\,\frac{d_2}{d_1}, \qquad Q_\beta = \frac{1}{p}, \tag{15}$$

where

$$\begin{aligned}
a &= \frac{\varkappa_0}{\varkappa_1 - \varkappa_0} - b, \qquad b = \frac{\mu_0}{\mu_1 - \mu_0}, \\
d_1 &= 3b + 2(S_{1111} - S_{1133} - S_{3311} - S_{1212} + S_{3333}), \\
d_2 &= b^2 + b(2S_{1111} - 2S_{1212} + S_{3333}) - 2(S_{1133}S_{3311} - S_{1111}S_{3333} + S_{1212}S_{3333}), \\
p &= \frac{1}{5}\left[\frac{4(b + S_{1212} + S_{1313})}{(b + 2S_{1212})\,(b + 2S_{1313})} + \frac{3(a+b) + 4S_{1111} + 2S_{1133} - 4S_{1212} + 2S_{3311} + S_{3333}}{ad_1 + 3d_2}\right],
\end{aligned} \tag{16}$$

with direction-3 representing the symmetric axis of the spheroid.

When the inclusions are spherical, both L_{PCW} and L_{MT} coincide, as expected, and they are the HS lower bounds if the matrix is the softer phase. When the inclusions are the randomly oriented flat disks with the aspect ratio $w = 0$ $(S_{3333} = 1, S_{3311} = S_{3322} = \nu_0/(1-\nu_0)$, $S_{3131} = S_{3232} = 1/2)$, the MT moduli coincide with the HS upper bounds (if the matrix is the softer phase), and the PCW moduli yield

$$\begin{aligned}
\varkappa_{PCW} &= \varkappa_0 + c_1 \Big/ \left[\frac{\varkappa_1 + \varkappa_1^*}{(\varkappa_1 - \varkappa_0)\,(\varkappa_0 + \varkappa_1^*)} - \frac{c_1}{\varkappa_0 + \varkappa_0^*}\right], \\
\mu_{PCW} &= \mu_0 + c_1 \Big/ \left[\frac{\mu_1 + \mu_1^*}{(\mu_1 - \mu_0)\,(\mu_0 + \mu_1^*)} - \frac{c_1}{\mu_0 + \mu_0^*}\right],
\end{aligned} \tag{17}$$

where

$$\varkappa_r^* = \frac{4}{3}\,\mu_r, \qquad \text{and} \qquad \mu_r^* = \frac{\mu_r(9\varkappa_r + 8\mu_r)}{6(\varkappa_r + 2\mu_r)}. \tag{18}$$

This pair of moduli actually lies above the HS upper bounds, but as the allowable range of c_1 at $w = 0$ is equal to zero, they cannot be used at all.

Indeed for consistency with the hypothesis of impenetrability of the inclusions, it is important to observe the safe range of the volume concentration c_1 at a given w, as stated by Ponte Castañeda and Willis [1]:

$$c_1 \leq w \quad \text{if} \quad w \leq 1 \,; \qquad \text{and} \qquad c_1 \leq (1/w)^2 \quad \text{if} \quad w \geq 1 \,. \tag{19}$$

Within this range, the spheroids Ω_d will completely enclose the inclusion, and the calculated moduli will always stay inside the bounds. Outside this range, such a consequence is not guaranteed. Thus for the limiting case of discs, one can only work with the disc (or crack) density parameters (with $w \to 0$ instead of $w = 0$).

To shed some light on where the MT moduli stand in light of the PCW moduli, we have plotted in Figs. 1 and 2 the effective bulk and shear moduli of the composite with the aspect

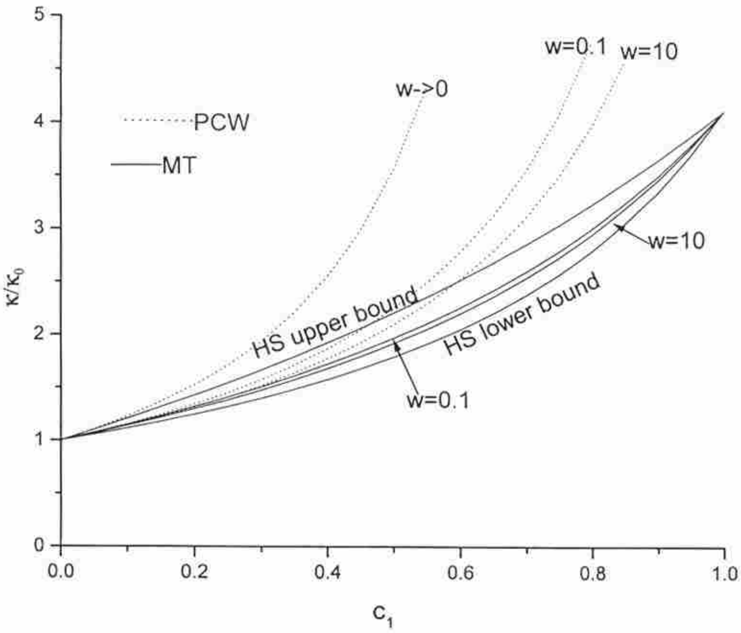

Fig. 1. Effect of inclusion shape on the bulk modulus of the isotropic composite with randomly oriented spheroidal inclusions: PCW and MT estimates, and HS bounds

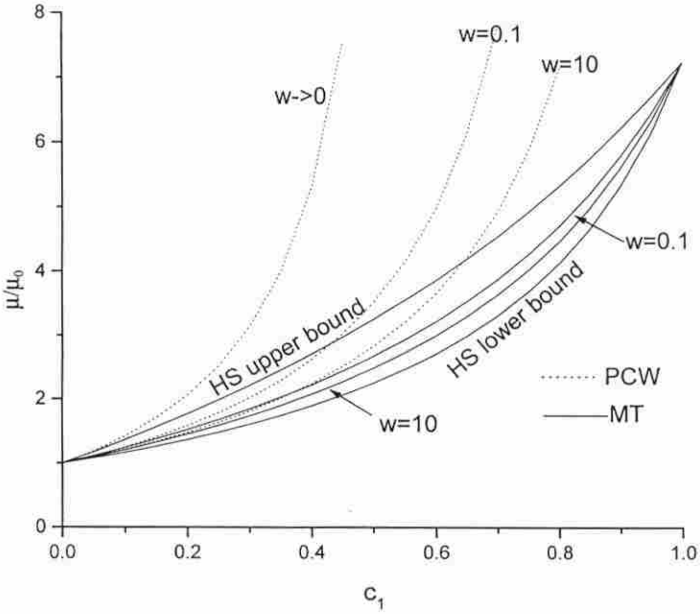

Fig. 2. Effect of inclusion shape on the shear modulus of the isotropic composite with randomly oriented spheroidal inclusions: PCW and MT estimates, and HS bounds

ratios $w = 0, 0.1$, and 10, along with the HS bounds. The material constants used here are $E_0 = 70$ GPa, $\nu_0 = 0.3$, and $E_1 = 468$ GPa, $\nu_1 = 0.18$. The predictions by the PCW method are found to be consistently higher than the MT method, regardless of the inclusion shape. The MT moduli, as already demonstrated in Tandon and Weng [9], all stay inside the bounds. The PCW moduli always stay inside the bounds within the allowable range of c_1. The moduli do not go outside the bounds immediately when c_1 goes beyond this range; for instance with $w = 0.1$ the bulk modulus does not go outside the bound at $c_1 = 0.1$ but stays inside it until $c_1 = 0.46$, and with $w = 10$ it does not go out at $c_1 = 0.01$ until $c_1 = 0.59$. These results suggest that the range provided in (19) may well be too "safe", or too conservative. In reality, the inclusions – especially needles – could still exist separately from contacting or penetrating into each other far beyond this range.

The fact that the MT moduli always stay inside the bounds is not to be interpreted that it is a superior theory. In fact it is impossible to conceive a microstructure with randomly oriented flat discs ($w = 0$) that they will not penetrate into each other, even at a dilute concentration.

4 Plasticity of the two-phase composite

The explicit bulk and shear moduli of the composite given by both theories are particularly suitable for the evaluation of the effective stress of the ductile matrix through the method proposed by Suquet [15] and Hu [18]. In essence, the methods of Castañeda [14], Suquet [15], Tandon and Weng [16], and Qiu and Weng [17] in conjunction with Hu [18] all make use of a linear comparison composite and deliver the same results for the overall stress-strain relations of the system. Here we follow the approach outlined in [17], [18] to calculate the elastoplastic behavior of the two-phase isotropic composite when the linear effective moduli are given by the PCW and MT methods, respectively.

In the composite system the effective stress of the heterogeneously deformed matrix can be defined directly as the volume average of the local effective stress, as [17]

$$\sigma_e{}^2 = < \sigma_e{}^2(x) > = \frac{3}{2} < \mathrm{s}(x)\,\mathrm{s}(x) > , \tag{20}$$

where x is the position vector, and s is the deviatoric stress tensor. This effective stress can be evaluated from the variation of the effective secant compliances tensor M_s of the composite with respect to the variation of its secant shear modulus $\mu_0{}^s$ by [18]

$$\sigma_e{}^2 = \bar{\boldsymbol{\sigma}} \left(-\frac{3\mu_0{}^{s2}}{1 - c_1} \frac{\partial M_s}{\partial \mu_0{}^s} \right) \bar{\boldsymbol{\sigma}} , \tag{21}$$

where $\bar{\boldsymbol{\sigma}}$ is the externally applied stress tensor of the composite.

Under a pure tensile loading $\bar{\sigma}$, it follows that

$$\sigma_e{}^2 = \frac{3\mu_0{}^s}{(1 - c_1)\, E_s{}^2} \frac{\partial E_s}{\partial \mu_0{}^s} \bar{\sigma}^2 , \tag{22}$$

in terms of E_s, the effective secant Young's modulus of the system.

This stress is to be used in the constitutive equation

$$\sigma_e = \sigma_y + h \cdot (\varepsilon_e{}^p)^n \tag{23}$$

to determine the magnitude of the effective plastic strain $\varepsilon_e{}^p$. Here, σ_y, h, and n are the tensile yield stress, strength coefficient and work-hardening exponent, in turn. The secant shear modulus is related to the secant Young's modulus $E_0{}^s$ and secant Poisson's ratio $\nu_0{}^s$, through

$$\mu_0{}^s = \frac{E_0{}^s}{2(1+\nu_0{}^s)}, \qquad E_0{}^s = \left[\frac{1}{E_0} + \frac{\varepsilon_e{}^p}{\sigma_y + h\cdot(\varepsilon_e{}^p)^n}\right]^{-1}, \qquad \nu_0{}^s = \frac{1}{2} - \left(\frac{1}{2} - \nu_0\right)\frac{E_0{}^s}{E_0}. \quad (24)$$

These secant moduli are to be identified with the elastic moduli of the matrix in the preceding sections for the evaluation of M_s (or M there).

At a given applied stress $\bar{\boldsymbol{\sigma}}$, the homogenized effective stress of the matrix, its secant moduli, and the effective secant compliance need to be evaluated iteratively so that the values of $\sigma_e, \varepsilon_e{}^p, \mu_0{}^s$ and M_s are consistent with one another. For a more detailed exposition of this method, one may refer to [17], [18].

Once M_s is known, the overall strain tensor of the composite follows as

$$\bar{\boldsymbol{\varepsilon}} = M_s \bar{\boldsymbol{\sigma}}. \quad (25)$$

By increasing the applied stress, the entire stress-strain curve of the system can be obtained.

The difference in the PCW and MT predictions lies in the effective secant compliances tensor of the composite M_s, or in the tensile case the secant Young's modulus E_s. To illustrate the difference of their predictions at various inclusion shapes, we have applied both to calculate the tensile stress-strain behaviors of a composite at $c_1 = 0.2$. In these calculations we have kept the previous elastic constants and used the plastic properties of an aluminum matrix [21], [22]: $\sigma_y = 250$ MPa, $h = 173$ MPa, and $n = 0.455$. The calculated nonlinear stress-strain curves are shown in Fig. 3. As in the elastic case, the predicted elastoplastic behaviors by the PCW method are again higher than the MT method.

To cast the predictions of both methods in some experimental perspective, we have also calculated the tensile behavior of a silicon-carbide/aluminum system tested by Yang et al.

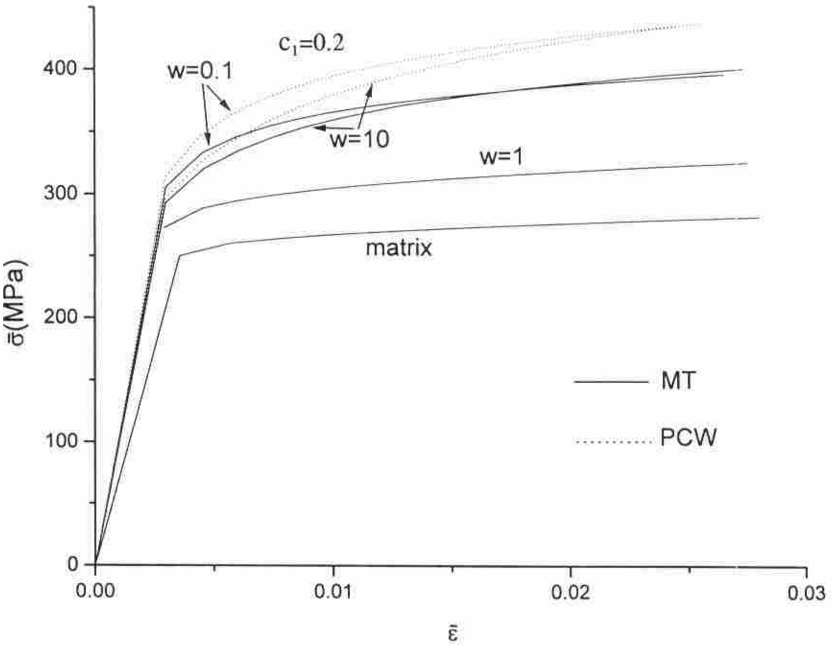

Fig. 3. Effect of inclusion shape on the nonlinear stress-strain relations of an isotropic composite with randomly oriented spheroidal inclusions: PCW and MT estimates

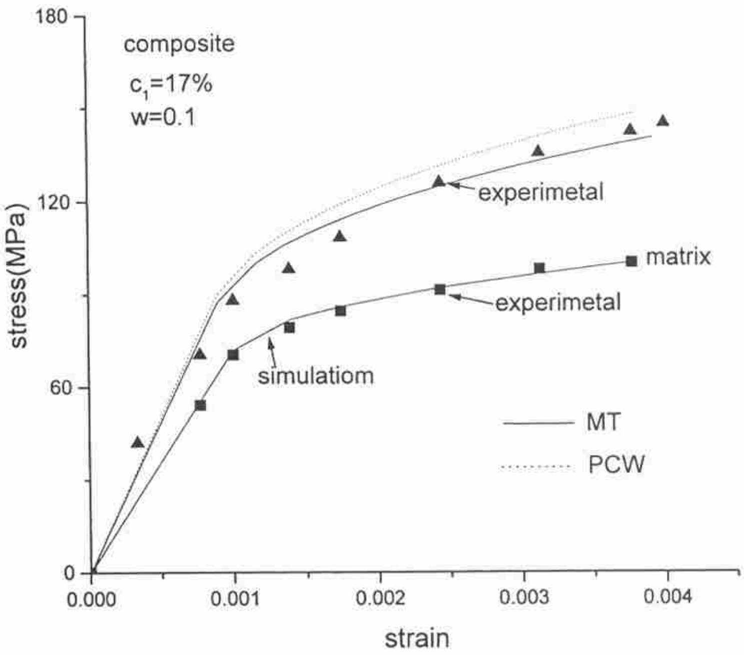

Fig. 4. Experimental comparison of the PCW and MT estimates with a silicon carbide/aluminum composite containing randomly oriented discs with an average aspect ratio $w = 0.1$

[23]. This system contained approximately 17% of silicon discs with an average aspect ratio of $w = 0.1$. The properties of the constituents in this case are: $E_1 = 490$ GPa, $\nu_1 = 0.17$; $E_0 = 68.3$ GPa, $\nu_0 = 0.33$, $\sigma_y = 70$ MPa, $h = 475$ MPa, and $n = 0.455$. The calculated curves by the two theoretical models are shown in Fig. 4, along with their experimental data for both the composite and the matrix. In view of the fact that the microstructure of the real system is rather complicated (e.g., the precise ellipsoidal shapes and the separation of inclusions), the predictions by both approaches can be said to lie within a reasonable range of accuracy.

5 Possibility for the MT model to be identified with a PCW microstructure

With aligned inclusions, Weng [13] and Ponte Castañeda and Willis [1] have proved that the MT model is identifiable with the microstructure of Willis [4], in which the distribution function of the inclusions is identical to the inclusion shape itself. In this final section, we ask: Is the MT model identifiable with the PCW microstructure when the inclusions are randomly oriented?

The discussion in [1] and the foregoing comparison have clearly demonstrated that, when the distribution function of inclusions is defined by an isotropic function or a sphere as represented by the white circles in Fig. 5a, the PCW model is distinctly different from the MT model. The other possible distribution function that can also give rise to an overall isotropy is one that takes the shape of the oriented inclusion itself, as sketched in Fig. 5b. Such an orientation-dependent distribution will bear a similar structure as in the 1-D aligned case when MT coincides with Willis [4]. With it, it appears quite possible that the corresponding PCW moduli could coincide with the MT moduli.

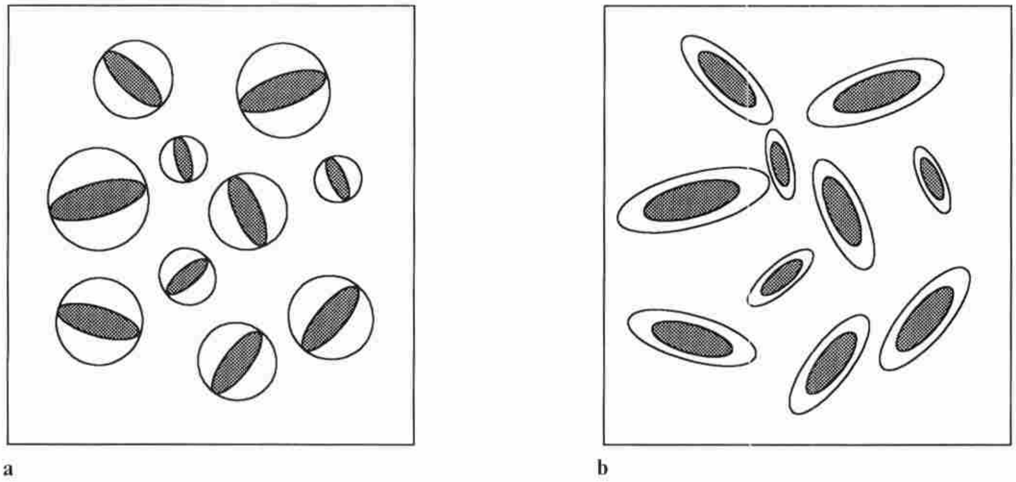

Fig. 5a. Spherical distribution and **b** ellipsoidal distribution of randomly oriented inclusions

We first explore whether the PCW formulation with such a distribution function would indeed give rise to the MT moduli. In this case $\Omega_d{}^{rs} = \Omega^r$ (the superscript r refers to the r-th oriented inclusion), and this leads to $P_d^{rs} = P_i{}^r$. In the local oriented coordinates, it has $P_i{}^r = P$ (all the inclusions have the same form). As such, the PCW moduli tensor, denoted by L'_{PCW}, becomes

$$L'_{PCW} = L_0 + c_1[I - c_1 < TP >]^{-1} < T > . \tag{26}$$

Furthermore, with the additional relations between T and Q, and P and S, and the isotropy of L_0, it can be recast into

$$L'_{PCW} = L_0\{I + c_1[< Q >^{-1} - c_1 < Q >^{-1} < QS >]^{-1}\} . \tag{27}$$

The orientational average on QS – in light of the identity (9) – operates only on Q. After some algebra it turns into

$$L'_{PCW} = L_0\{I + c_1[(1 - c_1) < Q >^{-1} + c_1(L_1 - L_0)^{-1}L_0]^{-1}\} = L_{MT} . \tag{28}$$

That is, if the distribution function of an oriented ellipsoid is taken to be identical to its own shape and orientation, the MT moduli can be derived from the PCW formulation. This outcome is consistent with that in the aligned case.

However, by taking the distribution function of an oriented inclusion to be identical to its own shape, it implies that $\Omega_d{}^{rs} = \Omega^r$. This would also imply that $\Omega_d{}^{sr} = \Omega^s$. As $\Omega^r \neq \Omega^s$ in the global coordinates, one finds that $P_d{}^{rs} \neq P_d{}^{sr}$. The joint probability density function is thus not symmetric, and this is, unfortunately, in violation to its basic definition.

One is led to conclude that, with randomly oriented ellipsoidal inclusions, the MT model cannot be realized from the PCW microstructure.

It remains an open question whether the microstructure depicted in Fig. 5b can be described by another formulation.

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