A two way particle mapping for calculation of the shear modulus of a spherical inclusion composite with inhomogeneous interphase

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Abstract

Based on the Mori–Tanaka method and a replacement scheme, a pair of coupled first order differential equations which model the shear modulus of a particulate composite with inhomogeneous interphase are derived. However, the results derived are not exact since the Mori–Tanaka method is not exact for the shear problem. An improved model is therefore proposed which utilises the generalised self consistent scheme for a spherical inclusion that is surrounded by a hypothetical homogeneous interphase layer. To find the properties of this hypothetical interphase layer a mapping of a homogeneous particle onto a two phase composite is utilised. The results are then

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presented for a simple power law profile and are shown to be consistent with the conclusions of Shen and Li [Int. J. Solids and Struct., 40, 2003, 1393–1409].

Contents

1 Introduction

A material, such as a polymer, that has some sort of reinforcing filler (or inclusion) embedded within it is known as a polymer composite. Fillers are added to the polymer with the aim of either improving the mechanical, thermal or electrical properties of the polymer or of improving a combination of these properties. The resulting composite material has many advantages over the original polymer and is therefore more suitable for particular applications than other more traditional materials.

Of particular importance on the overall mechanical properties of a composite is the interphase which is a three dimensional region immediately surrounding the inclusion. The bonding between the matrix and the inclusion occurs across this region and the stiffness properties of this region differ from that of the matrix and the inclusion.

Earlier work modeling the mechanical properties of composite materials ignored the effects of an interphase and are considered as two phase composites. The shear modulus of a two phase composite consisting of isotropic spherical inclusions surrounded by an isotropic matrix has been derived by Weng [2] using the Mori–Tanaka method [3] and a different expression has also been derived by Christensen & Lo [4] using the Generalised Self Consistent (GSC) Scheme. The Generalised Self Consistent method provides the exact solution to the shear problem.

In this work the shear modulus for a two phase composite containing spherical inclusions as derived by Weng [2] using the Mori–Tanaka method is used, to account for an inhomogeneous interphase region surrounding each inclusion. A replacement method is used as has been done for the bulk modulus case [5]. The results for any profile of the interphase region are generalised by deriving a coupled pair of first order differential equations. The differential equations are then solved exactly for the same power law profile given in [5], giving a closed form solution for the shear modulus. Since the differential equations that are derived are based on the Mori–Tanaka solution for the shear modulus which is only an approximation, an improved model based on the generalised self consistent method incorporating a homogeneous interphase is proposed. The results for the improved model are close to the Mori–Tanaka interphase model except for certain special cases which shall be discussed later.

2 The Mori–Tanaka interphase model

In this section we a model for the shear modulus of a composite with an inhomogeneous interphase is derived. The shear modulus of a two phase composite containing isotropic spherical inclusions surrounded by an isotropic matrix, as given by the Mori–Tanaka method, is

$$\mu = \mu_m + c\left[\frac{1}{\mu_p - \mu_m} + \frac{6}{5}\frac{(1-c)(\kappa_m + 2\mu_m)}{\mu_m(3\kappa_m + 4\mu_m)}\right]^{-1}, \tag{1}$$

where c is the volume fraction of the inclusions, μ_p is the shear modulus of the inclusion, and κ_m and μ_m are respectively the bulk and shear modulus of the matrix.

Consider an interphase region of finite size surrounding each inclusion as in [5]. The properties of the interphase are assumed to vary as a function of the radial distance from the centre of the inclusion. These functions are again assumed to be smooth, bounded and continuous. The radius of the inclusion is assumed to have length a and the thickness of the interphase is $(b-a)$.

The inclusion and interphase together are modeled as forming a new, effective spherical particle of radius b. It shall also be assumed that the inclusions are well spaced apart and that the interphase regions do not overlap. Note also that for the composite with inhomogeneous interphase, we denote the volume fraction of inclusions relative to all phases by d_0.

By splitting the interphase region into different layers or regions as in [5], the particle and first layer of interphase is modeled as a new effective spherical particle. Equation (1) is then re-applied using this new effective spherical particle as the inclusion phase and the next layer of interphase as being equivalent to the matrix phase. This technique is known as the replacement method and was proposed by Qiu & Weng [6] and Hashin [7]. Equation (1) may be re-applied over and over until all the layers have been used.

The interphase region may be split into n concentric layers causing a partition $\mathcal{P}$ of $[a, b]$ into n subintervals [5]. The lengths of these subintervals need not be the same and any point within each subinterval given by $\xi_i \in [x_{i-1}, x_i]$ may be chosen, where x represents the radial distance from the centre of the inclusion. Then everything proceeds here analogously to the bulk modulus case [5].

The effective shear modulus μ_i of the particle up to the ith layer is approximated by

$$\mu_i = \mu(\xi_i) + d_i \left[\frac{1}{\mu_{i-1} - \mu(\xi_i)} + \frac{6}{5} \frac{(1 - d_i)(\kappa(\xi_i) + 2\mu(\xi_i))}{\mu(\xi_i)(3\kappa(\xi_i) + 4\mu(\xi_i))} \right]^{-1} , \qquad (2)$$

where $d_i = (x_{i-1}/x_i)^3$, $1 \le i \le n$, $\xi_i \in [x_{i-1}, x_i]$ and $\mu_p = \mu_0$. $\kappa(x)$ and $\mu(x)$ are functions describing the properties of the interphase region such that $x \in [a, b]$ and μ_{i-1} is an approximation to the shear modulus of the inner composite sphere.

The aim is to find the effective shear modulus, μ_E, of the inclusion and whole interphase region:

$$\mu_E = \lim_{n \to \infty} \mu_n ,$$

where μ_n is found by solving the recurrence relation (2).

The effective shear modulus of the inclusion and interphase is

$$\mu_E = \frac{\mu_0 S(b) + T(b)}{\mu_0 U(b) + V(b)} . \qquad (3)$$

where $S(x)$ and $U(x)$ are the solutions of a pair of coupled first order linear differential equations:

$$S'(x) = -\frac{3}{5x} \left(\frac{9\kappa(x) + 8\mu(x)}{3\kappa(x) + 4\mu(x)} \right) S(x) + \frac{3\mu(x)}{5x} \left(\frac{9\kappa(x) + 8\mu(x)}{3\kappa(x) + 4\mu(x)} \right) U(x) , \qquad (4)$$

$$U'(x) = \frac{18}{5x\mu(x)} \left(\frac{\kappa(x) + 2\mu(x)}{3\kappa(x) + 4\mu(x)} \right) S(x) - \frac{18}{5x} \left(\frac{\kappa(x) + 2\mu(x)}{3\kappa(x) + 4\mu(x)} \right) U(x) , \qquad (5)$$

where $S(a) = 1$, $U(a) = 0$ and $x \in [a, b]$. A detailed derivation of these equations is given in [10].

The functions $T(x)$ and $V(x)$ are found by solving equations (4) and (5) after replacing S with T and U with V, where $T(a) = 0$, $V(a) = 1$ and $x \in [a, b]$. Therefore, only one set of equations needs to be solved with appropriate care taken when accounting for the boundary conditions.

The shear modulus of the composite can then easily be found by substituting $\mu_p = \mu_E$ in equation (1) and letting $c = d_0 b^3/a^3$.

3 The improved model

3.1 A reverse particle mapping

The above results represent a mapping of an inclusion with a surrounding interphase onto an effective homogeneous particle with different size and properties to the original inclusion. Therefore, other micromechanics models which have an explicit solution for the shear modulus may be incorporated into the present results. For example, in the Generalised Self Consistent Scheme, the shear modulus is given by the solution of a quadratic equation [4]. This result is useful in that it enables us to test the effect of the inhomogeneous region using other micromechanics models. This was the approach used recently by Shen & Li [1] who checked their results against finite element computations. It was found that their model was rather accurate when the properties of the interphase vary between those of particle/fibre and matrix but was unsatisfactory when the interphase was much harder than both particle/fibre and matrix, and the matrix was harder than the inclusion.

The GSC method of Christensen & Lo [4] gives the exact solution to the two phase shear problem whereas the Mori–Tanaka solution is only an approximation and consequently there is an error in the current method.

Wang & Jasiuk [9] solved the shear modulus problem exactly for the power law profile using the GSC method by solving a partial differential equation for the displacement of the material that is subjected to shear strain at infinity. Use of this approach for other profiles may be problematic due to the complexity of the partial differential equation governing the displacement.

An alternative approach is therefore proposed where the results of Theocaris [8] are utilised. Theocaris [8] derives the shear modulus of a particulate composite with homogeneous interphase using the GSC method of Christensen & Lo [4].

In order to estimate the shear property of the interphase a reverse mapping of the homogeneous properties of the effective particle consisting of inclusion and interphase onto a two phase composite is utilised as shown in Figure 1. Note that perfect bonding is assumed to exist between the phases. This can be achieved by solving the following two simultaneous equations for κ_i and μ_i:

$$\kappa_E = \kappa_i + \frac{a^3}{b^3}\left[\frac{1}{\kappa_p - \kappa_i} + \frac{3(1-\frac{a^3}{b^3})}{3\kappa_i + 4\mu_i}\right]^{-1}$$

$$\text{and} \qquad \mu_E = \mu_i + \frac{a^3}{b^3}\left[\frac{1}{\mu_p - \mu_i} + \frac{6}{5}\frac{(1-\frac{a^3}{b^3})(\kappa_i + 2\mu_i)}{\mu_i(3\kappa_i + 4\mu_i)}\right]^{-1},$$

where the subscript i denotes the interphase. Note that κ_E and μ_E are given by [5] and (3) respectively. The solution to these two simultaneous equations gives only one physically realistic solution, that is $\kappa_i > 0$ and $\mu_i > 0$. The remaining solutions may be discarded.

Therefore, by utilizing the above values for κ_i and μ_i and then solving the shear problem with a homogeneous interphase using the GSC method, an improvement in the accuracy of the results should be achieved.

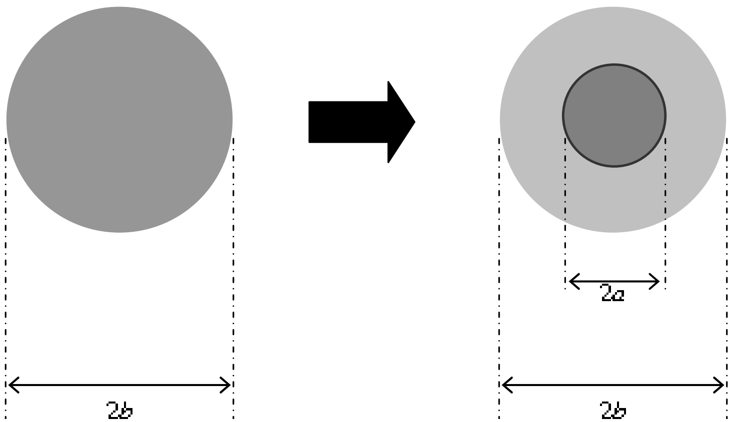

Figure 1: A mapping of a homogeneous particle consisting of inclusion and interphase onto a two phase composite.

3.2 The GSC method with a homogeneous interphase

In the original model, a composite sphere or cylinder consisting of the inclusion and a concentric shell with the property of the matrix, is embedded in a surrounding material which has the unknown properties of the composite material. Theocaris [8] extended this model by incorporating a homogeneous interphase region surrounding the inclusion. A detailed description of this method is also given by Lombardo [10].

Everything proceeds similarly to the case where no interphase region is present [4]. The solution involves solving the equations of equilibrium in each of the homogeneous phases when the composite is subjected to shear strain at infinity. The unknowns which appear in these solutions are found by ensuring continuity of stresses and displacements at each interface. A result obtained by Eshelby [11] is also used to eliminate one of the unknown constants. The solution to the remaining unknown constants is found by solving a 12×12 matrix system as opposed to an 8×8 matrix system that occurs when the interphase is neglected [4].

4 Results

To check whether the model is satisfactory, a simple power law function as in [5] is considered. Shen & Li concluded in their work that their model for the shear modulus was not satisfactory when the interphase is much harder than the matrix and the particle inclusion, and the inclusion softer than the matrix. Since their model, like the current model, is based on the Mori–Tanaka solution for the shear modulus, the present model will reflect the same behaviour. However, it is worthwhile for such cases to consider the behaviour of the improved model which employs the generalised self consistent method.

A comparison between the improved model and the Mori–Tanaka interphase model is shown below by considering the following variations in the interphase properties given in Figures 2 and 3. The material properties used were $\kappa_m = 22$, $\mu_m = 11$, $\kappa_p = 14$ and $\mu_p = 3$ and the interphase region was assumed to have a thickness of 25% of the radius of inclusion. Also, various values of J (an interphase parameter which measures the modulus at the surface of the inclusion relative to the modulus of the matrix), were chosen such that the interphase properties are harder than both inclusion and matrix, a similar case considered in the work of Shen & Li [1].

For such an interphase profile the shear modulus as a function of inclusion concentration using the Mori–Tanaka interphase model and the improved model are plotted and are given respectively in Figures 4 and 5.

Figures 4 and 5 show that the larger the value of J, the greater the variation in the Mori–Tanaka interphase model and the improved model. This behaviour is also reflected in the work of Shen & Li [1] who used a damage parameter to change the properties of the interphase region. This damage parameter is analogous to the parameter J. They measured the change in the strain energy based on the present model to finite element computations. For the shear modulus, they showed that the larger the damage parameter, the smaller the error in the strain energy between the present method and

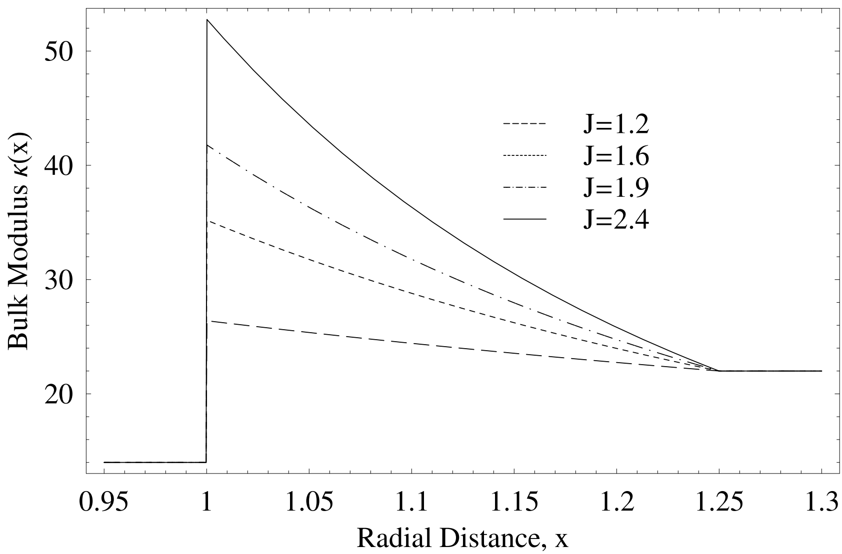

Figure 2: The bulk modulus as a function of the radial distance, x.

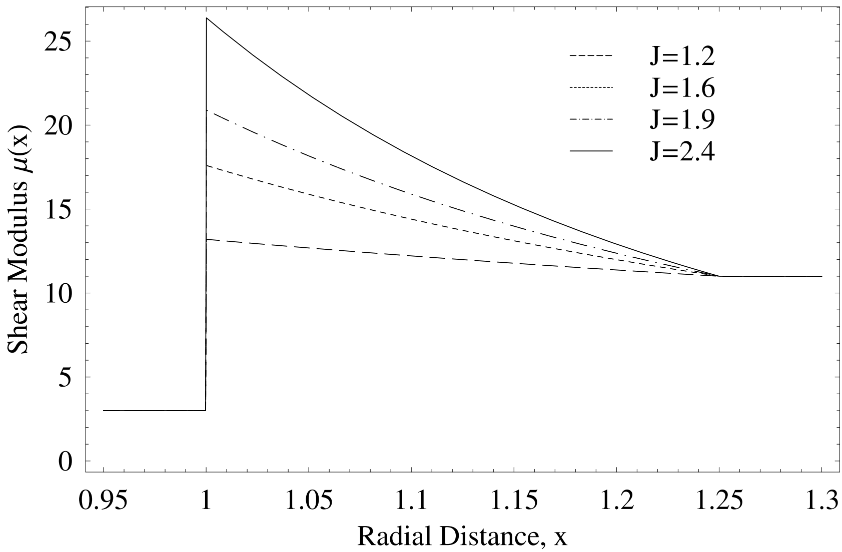

FIGURE 3: The shear modulus as a function of the radial distance, x.

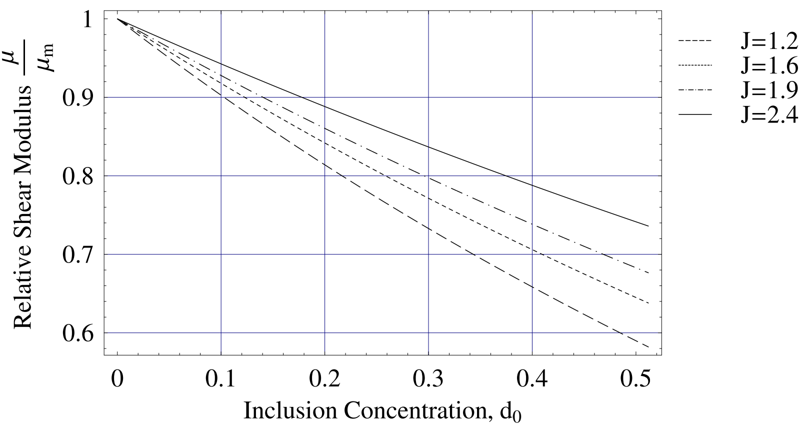

FIGURE 4: The relative shear modulus of a composite as a function of inclusion concentration for various values of J, plotted using the Mori–Tanaka interphase model.

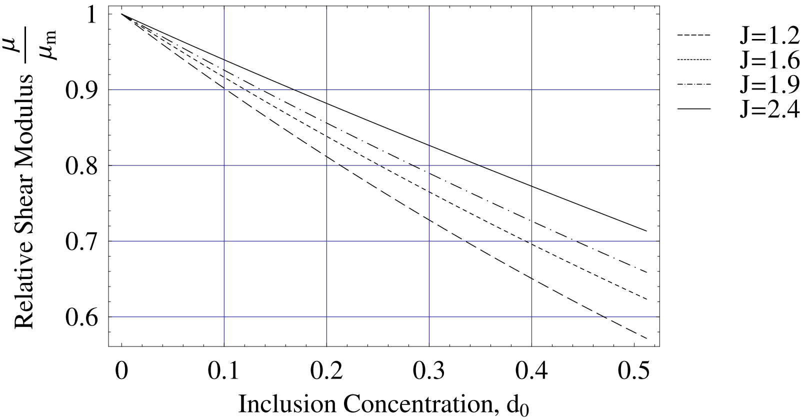

Figure 5: The relative shear modulus of a composite as a function of inclusion concentration for various values of J, plotted using the improved GSC homogeneous model.

the finite element computations, a behaviour that is reflected in the current work.

5 Conclusion

An approximation was obtained to the shear modulus of a particulate composite with an inhomogeneous interphase using a result obtain by Weng [2] for a two phase composite based on the Mori–Tanaka method. As in the bulk modulus case, an exact solution for the effective shear modulus of the inclusion and interphase using power law profile was obtained from a coupled pair of differential equations. To account for the fact that the Mori–Tanaka solution is not exact, the generalised self consistent method of Christensen and Lo [4] was employed. This was achieved by doing a reverse mapping of the homogeneous particle consisting of inclusion and interphase back onto a two phase composite. Such a mapping made it possible to estimate the equivalent homogeneous property of the interphase. The GSC method was then modified to account for this homogeneous interphase region surrounding the inclusion. The accuracy of the improved model seems to depend on how good the estimate is of the equivalent homogeneous properties of the interphase since the method is exact after these properties are known. It is not known how accurate the method is that we use to measure the equivalent homogeneous properties of the interphase. However, the results reflect the behaviour that is expected. That is, when the properties of the interphase vary between inclusion and matrix, then the difference between both models is small or hardly perceived. However, when the inclusion is softer than the matrix and the interphase is harder than both, then the results show a clear difference between both models, a result that is reflected in the work of Shen & Li [1].

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