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A unified scheme for prediction of effective moduli of multiphase composites with interface effects. Part I: Theoretical framework

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Abstract

In this part of the two-part paper, we present a unified theoretical framework to predict the effective moduli of multiphase composites containing spherical particles or cylindrical fibres with various interface effects. This framework is based upon a replacement procedure and the generalized self-consistent prediction of the effective moduli. However, both of the replacement procedure and the generalized self-consistent prediction are different from the conventional ones in that the former is implemented in terms of an energy equivalency condition to calculate the elastic constants of the equivalent particles or fibres, and the latter is based upon the Eshelby equivalent inclusion method in an average sense for the three-phase configuration. Using this replacement procedure, the expressions for the moduli of the spherical particles and cylindrical fibres with the linear-spring interface effect, the interface stress effect and the interphase model are presented. It is shown in a companion paper (Part II) that this scheme, together with the decoupled formulas for the generalized self-consistent prediction of the effective moduli of multiphase composites, can give simple and accurate predictions of the effective moduli.

Keywords: Multiphase composites; Effective moduli; Interface effects; Linear-spring model; Interface stress model; Interphase model; Generalized self-consistent method

1. Introduction

Interfacial bonding condition is one of the important factors that control the local elastic fields and the overall properties of composites and polycrystalline materials. In many cases, imperfect interfacial bonding may exist in these materials (e.g. Theocaris, 1987), and the interfacial bonding condition may greatly affect their properties. For example, grain boundary sliding in polycrystalline and granular media can be observed even at room temperature (Mura and Furuhashi, 1984). It is found that fornanocrystalline materials, the macroscopically imposed deformation is accommodated by the grain-boundary sliding and separation (Schiøtz et al., 1998; Wei and Anand, 2004). Zhang and Hack (1992) have previously pointed out that the softening of grain boundaries is not only important in

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nanocrystalline materials but also in conventional materials where grain boundary cavitation and intergranular fracture may occur. In the literature, two kinds of model are often used to simulate the properties of interface regions in composites and polycrystalline materials. The first kind of model can be referred to as interface models in which displacement and/or stress discontinuities are assumed to exist at an interface. Interface models include the linear-spring interface model and the interface stress model. The second kind is the interphase model which describes the interface region as a layer, called an interphase, between the inhomogeneity and matrix. The elastic moduli of the interphase are different from those of the matrix and inhomogeneity, and can be uniform or variable. Perfect bonding is generally assumed to prevail at both the matrix/interphase and interphase/inhomogeneity interfaces.

Within the formalism of interface and interphase models, extensive researches have been devoted to the elastic fields and effective properties of conventional particle- and fibre-reinforced composites (e.g. Walpole, 1978; Aboudi, 1991; Karihaloo and Viswanathan, 1988a,b; Hashin, 1991; Qu, 1993; Zhong and Meguid, 1997; Duan et al., 2005a,b,c,d, among others). Recently, based upon the atomic simulation of Schiøtz et al. (1998), Jiang and Weng (2004) have proposed a three-phase model to predict the overall properties of nanocrystalline materials, in which the grain-boundary region is simulated by an interphase between a grain and its surrounding material. On the other hand, considering that the grain-boundary region may be very thin, Wei and Anand (2004) developed an elastic–plastic interface model coupled with a crystal-plasticity model for the grain interior to simulate the overall response of nanocrystalline materials. The interface model can account for both reversible elastic and irreversible inelastic separation-sliding deformations at the interface. The elastic deformation is simulated by a linear-spring interface constitutive law. Tan et al. (2005a) have predicted the effective constitutive relations of composites containing particles with a piecewise linear cohesive law at the particle/matrix interface under hydrostatic tension. The interface law of Tan et al. (2005a,b) consists of three stages, namely, the linearly ascending stage (i.e. a linear-spring model), the linearly descending stage and the complete debonding stage. Therefore, the theories of Jiang and Weng (2004), Wei and Anand (2004), and Tan et al. (2005a,b) involve two typical models, namely, an interphase model and an interface model.

In this two-part paper, we propose a unified micromechanical scheme to predict the effective moduli of multiphase composites which consist of continuous matrices and discrete spherical or cylindrical inhomogeneities with various interface effects. This scheme is based upon a replacement procedure that replaces the spherical particles/fibres together with the interface/interphase by equivalent homogeneous particles/fibres. However, as will be further elaborated in Section 2, the present replacement procedure is different from the previous ones in that the effective elastic constants of the equivalent homogeneous particles/fibres are calculated in terms of an energy equivalency condition. Then the equivalent homogeneous particles/fibres are in turn incorporated into the three-phase generalized self-consistent model to predict the effective moduli of the composites. Unlike the classical generalized self-consistent method (GSCM, Christensen and Lo, 1979) where the elastic field is solved from the boundary-value problem, in this paper, the average stresses in the equivalent particles/fibres are solved by using the Eshelby equivalent inclusion method in a volume average sense. It is shown that while the obtained effective bulk moduli of the composites are identical to those obtained using the classical GSCM, the expressions for the effective shear moduli obtained from the new scheme is much simpler than those from the classical one. Moreover, as will be shown in Part II, when the interface effects are taken into account, some intrinsic length scales will emerge, and the effective properties of the composites will become dependent upon the characteristic size of the inhomogeneities. Therefore, we shall also show that the size-dependence of the properties can be nicely and accurately depicted by some scaling laws. Although the studies in the present paper are for composites with linear stress–strain responses, the results can be useful in the studies of the effective constitutive relations of nonlinear composites following the theoretical framework based upon the concept of "*linear comparison composites*", as demonstrated, for example, in the works of Ponte Castañeda and Suquet (1998), and Jiang and Weng (2004).

In this part of the two-part paper, the fundamental theoretical framework of the unified micromechanical scheme will be presented, and in Part II, the scheme will be demonstrated on various composites to show its applicability and accuracy. The scaling laws will also be presented in Part II.

2. Replacement procedure for inhomogeneities with interface effects

Various interface effects complicate predictions of the effective moduli of composites. The idea of the replacement method may be attributed to Hashin (1990), who studied the prediction of the effective moduli of a composite reinforced by fibres with the linear-spring interface effect. In order to calculate the effective moduli, Hashin (1990), while noting that the linear-spring interface model can be equivalent to a thin and compliant interphase, first used a layer of thin and compliant interphase to approximate the linear-spring interface effect. Then he calculated the moduli of the equivalent fibre consisting of a fibre and the thin interphase using the composite cylinder model. Finally, he embedded the equivalent fibre in an annulus of the matrix material of the composite, and calculated the effective moduli of this composite fibre using the composite cylinder model again. The moduli so-obtained are regarded as those of the original composite with the linear-spring interface effect. Hashin (1991) also used this method to obtain the bulk modulus of a particle-reinforced composite with the linear-spring interface model. Qiu and Weng (1991) used this replacement method to obtain the effective bulk modulus $\bar{\kappa}$ of a composite containing spherical particles with an interphase, and the longitudinal modulus $\overline{E}_{\mathrm{L}}$, the longitudinal Poisson ratio $\bar{\nu}_{\mathrm{L}}$, the longitudinal shear modulus $\bar{\mu}_{\mathrm{L}}$, and the transverse plane-strain bulk modulus $\bar{k}$ of a composite reinforced with aligned fibres with an interphase. Garboczi and Berryman (2001), and Zhong et al. (2004) developed differential effective medium theories based on a replacement method, which also maps the original particles together with the homogeneous and inhomogeneous interphases into equivalent homogeneous particles, to predict the effective moduli of composites containing interphases. Shen and Li (2005) presented several methods to convert spherical particles/fibres with an inhomogeneous interphase into homogeneous particles/fibres. Then the elastic constants of the homogeneous particles/fibres are incorporated into the Mori–Tanaka method to predict the effective moduli of the composites. In the work of Shen and Li (2005), the elastic constants of the equivalent homogeneous particles/fibres with an inhomogeneous interphase are calculated in several ways, e.g. the differential replacement method and the uniform replacement method.

In the above replacement methods, the elastic constants of the equivalent homogeneous particles/fibres are calculated essentially based upon the composite sphere/cylinder model, namely, by treating a particle/fibre together with the interphase as a composite independently. Moreover, the obtained expressions for the effective shear moduli of the composites reinforced by particles/fibres are usually very lengthy. In the literature, the interface stress effect has not been studied using a replacement method. Therefore, at present, there lacks a unified scheme to give simple and accurate predictions of the effective moduli of composites with various interface effects. As the effective moduli of a composite can be generally sought based upon the energy equivalency framework (Hill, 1963), therefore, in this paper, we propose a new replacement procedure based upon an energy equivalency condition to calculate the elastic constants of the equivalent homogeneous particles/fibres. This method, which is consistent with the energy equivalency framework, is different from those in the above-mentioned papers.

In this paper, we consider particle- or fibre-reinforced composites in which the interfaces are depicted by the linear-spring model (including free-sliding model), the interface stress model, and the interphase model, respectively. A common feature of these models is that the traction/displacement may be discontinuous across the interface region. Therefore, in this section, in order to give a general theoretical framework, we do not deal with any specific interface model; instead, we simply consider a generic imperfect interface where the traction/displacement undergoes a discontinuity across the interface, as shown in Fig. 1. In an effort

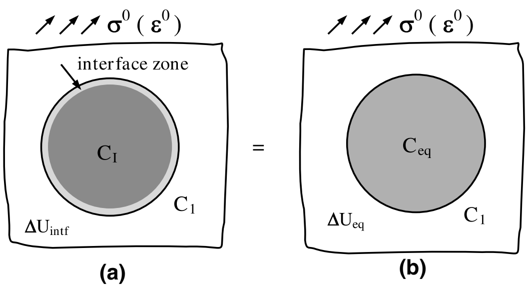

Fig. 1. A replacement procedure based on the energy equivalency condition. The energy change induced by embedding an inhomogeneity with the interface effect is ΔU_{intf} (a), and that induced by embedding the perfectly-bonded equivalent inhomogeneity is ΔU_{eq} (b).

to uncover the effect of the interface on the elastic properties, a replacement procedure based on an energy equivalency condition, which replaces the original particles/fibres with the interface effect by equivalent homogeneous particles/fibres, is presented. The equivalent homogeneous particles/fibres are then regarded as being perfectly bonded to the matrix, and then a micromechanical scheme can be used to estimate the moduli of the composites. Therefore, the key point is to obtain the moduli of the equivalent particles/fibres with the generic interface effect. In the following exposition, the terminology inhomogeneity refers to a particle or a fibre when it is not necessary to differentiate them.

The present replacement procedure is carried out in the following way. Consider a single inhomogeneity with the generic interface effect embedded in an infinite and otherwise homogeneous medium (matrix) with the stiffness tensor $\mathbf{C}_1$ (Fig. 1(a)). The remote stress (strain) is $\boldsymbol{\sigma}^0(\boldsymbol{\varepsilon}^0)$, and the stiffness tensor of the inhomogeneity is $\mathbf{C}_\mathrm{I}$. Generally, embedding the inhomogeneity with the interface effect in the medium will result in a change ΔU_intf of the elastic strain energy of the infinite medium compared with the energy of the homogeneous medium under the same stress (strain). Now, the inhomogeneity with the interface effect is replaced with an equivalent homogeneous inhomogeneity with an unknown stiffness tensor $\mathbf{C}_\mathrm{eq}$, which is, however, perfectly bonded to the matrix material. The unknown stiffness tensor $\mathbf{C}_\mathrm{eq}$ is determined by the energy equivalency condition that the change ΔU_eq of the elastic energy by embedding the equivalent inhomogeneity in the matrix material is equal to the original change ΔU_intf of the original inhomogeneity together with the interface effect, namely, $\Delta U_\mathrm{intf} = \Delta U_\mathrm{eq}$. Using the Eshelby formalism, the change ΔU_eq of the elastic energy can be easily obtained

$$\Delta U_\mathrm{eq} = \frac{V_\mathrm{eq}}{2}\mathbf{C}_1 : \boldsymbol{\varepsilon}^0 : [\mathbf{C}_1 : (\mathbf{C}_\mathrm{eq} - \mathbf{C}_1)^{-1} : \mathbf{C}_1 + \mathbf{C}_1 : \mathbf{S}^0]^{-1} : \mathbf{C}_1 : \boldsymbol{\varepsilon}^0 \quad (1)$$

where $\mathbf{S}^0$ is the classical interior Eshelby tensor (Eshelby, 1957), and V_eq is the volume of the equivalent inhomogeneity. In order to determine the stiffness tensor $\mathbf{C}_\mathrm{eq}$ of the equivalent inhomogeneity from the energy equivalency condition $\Delta U_\mathrm{intf} = \Delta U_\mathrm{eq}$, we need to calculate ΔU_intf for a specific interface model. This will be done for three kinds of interface effect in the next section.

3. Interface conditions and moduli of equivalent inhomogeneities

3.1. Interface conditions

In the following, we shall give the formulas to calculate the moduli $\mathbf{C}_\mathrm{eq}$ of the equivalent inhomogeneities for three kinds of interface effect. First, we summarize the expressions for the displacement/stress discontinuities for the considered interface effects.

3.1.1. Linear-spring model (LSM)

As mentioned in Section 1, the linear-spring interface model has been widely used to simulate the interface bonding in particle-reinforced composites (e.g. Hashin, 1991). Apart from being used to simulate the imperfect interfacial bonding or debonding (e.g. Tan et al., 2005a,b), this model can also be used to simulate a thin and compliant interphase (Hashin, 1991; Wei and Anand, 2004; Wang et al., 2005, etc.). The interface conditions for the linear-spring model can be written as

$$[\boldsymbol{\sigma}] \cdot \mathbf{n} = \mathbf{0}, \quad \boldsymbol{\alpha} \cdot [\mathbf{u}] = \boldsymbol{\sigma} \cdot \mathbf{n} \quad (2)$$

where $\mathbf{n}$ is the unit normal vector to the interface $\Gamma_{\mathrm{I}1}$ between the inhomogeneity and matrix, and $[\cdot] = (\mathrm{out}) - (\mathrm{in})$. $\boldsymbol{\alpha}$ is a second-order tensor, $\boldsymbol{\alpha} = \alpha_\mathrm{n}\mathbf{n}\otimes\mathbf{n} + \alpha_\mathrm{s}\mathbf{s}\otimes\mathbf{s} + \alpha_\mathrm{t}\mathbf{t}\otimes\mathbf{t}$. α_n, α_s and α_t represent the interface elastic parameters in the normal and tangential directions, respectively, and $\mathbf{s}$ and $\mathbf{t}$ represent the two orthogonal unit vectors in the tangent plane of the interface. It is seen that infinite values of these parameters imply vanishing interface displacement jumps and therefore a perfect bonding interface. At the other extreme, zero values imply vanishing interface tractions and therefore debonding of the adjoining media. Finite positive values of the interface parameters define an imperfect interface. As mentioned before, the linear-spring model can be used to simulate a thin and compliant interphase (Hashin, 1991; Wei and Anand, 2004; Wang et al., 2005). In this case, α_n, α_s and α_t can be expressed by the interphase modulus and interphase thickness. When the interphase is thin and compliant, namely, $t/R_\mathrm{I} \ll 1$, $E_\mathrm{c} \ll E_\mathrm{I}$, $\mu_\mathrm{c} \ll \mu_\mathrm{I}$, where E_c and μ_c are the Young and shear moduli of the interphase, respectively; E_I and μ_I are the Young and shear moduli of the inhomogeneity; R_I is the radius of the spherical inhomogeneity; and t is the interphase thickness (throughout this two-part paper, the parameters for the inhomogeneities (particles/ fibres) will be distinguished by the subscript I), α_n, α_s and α_t can be expressed as follows (Hashin, 1991; Wang et al., 2005):

$$\alpha_n = \frac{2\mu_c(1-\nu_c)}{t(1-2\nu_c)}, \quad \alpha_s = \alpha_t = \frac{\mu_c}{t} \tag{3}$$

where ν_c is the Poisson ratio of the interphase.

For the linear-spring model (LSM), the change of the elastic energy under the remote strain boundary condition $\mathbf{u}(S) = \boldsymbol{\varepsilon}^0 \cdot \mathbf{x}$ by embedding an inhomogeneity with the interface effect is (Benveniste, 1985)

$$\Delta U_{\text{intf}}^{\text{LSM}} = \frac{1}{2}\int_{\Gamma_{\text{I1}}} (\mathbf{n}\cdot\boldsymbol{\sigma}\cdot\mathbf{u}^0 - \mathbf{u}^1\cdot\boldsymbol{\sigma}^0\cdot\mathbf{n})\mathrm{d}\Gamma_{\text{I1}} \tag{4}$$

where Γ_{I1} denotes the interface area on the matrix side, and the superscript "1" denotes the quantity evaluated at Γ_{I1} on the matrix side. $\boldsymbol{\sigma}^0$ and $\mathbf{u}^0$ denote the stress and displacement in the homogeneous body made of the matrix only.

3.1.2. Interface stress model (ISM)

The effect of the surface/interface stress on the mechanical properties of solids has been studied by researchers in materials science and mechanics for many years (e.g. Shuttleworth, 1950; Gurtin and Murdoch, 1975; Nix and Gao, 1998; Müller and Saúl, 2004; Sun et al., 2004). The interest in this subject has intensified recently for its importance in the properties of nano-structured materials (e.g. Cuenot et al., 2004; Duan et al., 2005a,b,c; Shenoy, 2005; Dingreville et al., 2005). Recent expositions of the physical background of the interface stress model can be found in the works of Müller and Saúl (2004), Duan et al. (2005a,b), Dingreville et al. (2005), and Huang and Wang (in press). Duan et al. (2005a) have previously predicted the effective moduli of heterogeneous solids containing spherical inhomogeneities with the interface stress effect. In this paper, we formulate the prediction in the unified framework based upon the replacement procedure and the generalized self-consistent method. As will be shown, this scheme gives much simpler expressions of the effective moduli than the previous ones. Therefore, here, we only reproduce the necessary basic equations of the interface stress model. The displacement continuity condition and the generalized Young–Laplace equation of the interface stress model are

$$[\mathbf{u}] = \mathbf{0}, \quad \mathbf{n}\cdot[\boldsymbol{\sigma}] = -\nabla_S\cdot\boldsymbol{\tau} \tag{5}$$

where $\nabla_S\cdot\boldsymbol{\tau}$ denotes the interface divergence of a tensor field $\boldsymbol{\tau}$ (Gurtin and Murdoch, 1975). For an isotropic interface, the interface stress $\boldsymbol{\tau}$ is related to the interface strain $\boldsymbol{\varepsilon}^{\text{s}}$ by the constitutive relation

$$\boldsymbol{\tau} = 2\mu_s\boldsymbol{\varepsilon}^{\text{s}} + \lambda_s(\text{tr}\,\boldsymbol{\varepsilon}^{\text{s}})\mathbf{1} \tag{6}$$

where λ_s and μ_s are the interface moduli, and $\mathbf{1}$ is the second-order unit tensor in two-dimensional space. For a coherent interface, the interface strain $\boldsymbol{\varepsilon}^{\text{s}}$ is equal to the tangential strain in the abutting bulk materials. Similar to the linear-spring interface model, the interface stress model, apart from being used to simulate the excess of the bulk stress at an interface (e.g. cf. Müller and Saúl, 2004), can be used to accurately simulate a thin and stiff interphase (Wang et al., 2005). For the former case, the interface moduli may be obtained using atomistic simulations (e.g. Streitz et al., 1994; Shenoy, 2005). For the latter case, namely, for a thin and stiff interphase ($t/R_{\text{I}} \ll 1$, $E_c \gg E_{\text{I}}$, $\mu_c \gg \mu_{\text{I}}$), the interface moduli λ_s and μ_s in Eq. (6) are given by (Wang et al., 2005)

$$\lambda_s = \frac{2\mu_c\nu_c t}{(1-\nu_c)}, \quad \mu_s = \mu_c t \tag{7}$$

The change of the elastic energy under the remote strain boundary condition $\mathbf{u}(S) = \boldsymbol{\varepsilon}^0\cdot\mathbf{x}$ by embedding an inhomogeneity with the interface stress effect is (Duan et al., 2005b)

$$\Delta U_{\text{intf}}^{\text{ISM}} = \frac{1}{2}\int_{\Gamma_{\text{I1}}} (\mathbf{n}\cdot\boldsymbol{\sigma}^1\cdot\mathbf{u}^0 - \mathbf{u}\cdot\boldsymbol{\sigma}^0\cdot\mathbf{n})\mathrm{d}\Gamma_{\text{I1}} \tag{8}$$

3.1.3. Interphase model

The linear-spring model and interface stress model are all two-phase models in the sense that the interface region occupies a zero volume fraction in the composite, whereas, the interphase model is a three-phase one, consisting of the inhomogeneity, the interphase and the matrix. For the interphase model, perfect bonding conditions are usually assumed to prevail at both the inhomogeneity/interphase interface Γ_{Ic} and the interphase/matrix interface Γ_{c1}, i.e.

$$\mathbf{n}^k\cdot[\boldsymbol{\sigma}^k] = \mathbf{0}, \quad [\mathbf{u}^k] = \mathbf{0} \quad (k = 1, 2) \tag{9}$$

where the superscript $k = 1, 2$ represents the interfaces Γ_{Ic} and Γ_{c1}, respectively. $[\boldsymbol{\sigma}^k]$ and $[\mathbf{u}^k]$ represent the stress and displacement discontinuities at the interfaces Γ_{Ic} and Γ_{c1}. The energy change under the remote strain boundary condition $\mathbf{u}(S) = \boldsymbol{\varepsilon}^0\cdot\mathbf{x}$ for the interphase model is

$$\Delta U_{\text{intf}}^{\text{interphase}} = \frac{1}{2}\int_{\Gamma_{c1}} (\mathbf{n}_1 \cdot \boldsymbol{\sigma} \cdot \mathbf{u}^0 - \mathbf{u} \cdot \boldsymbol{\sigma}^0 \cdot \mathbf{n}_1)\mathrm{d}\Gamma_{c1} \tag{10}$$

where $\mathbf{n}_1$ is the unit normal vector to the interface Γ_{c1}.

3.2. Moduli of equivalent homogeneous spherical particles

For the linear-spring model and the interphase model, the bulk moduli of the equivalent spherical particles obtained by the present energy equivalency condition are the same as those obtained by the composite sphere model of Hashin (1991), and Qiu and Weng (1991), respectively. For the interface stress model, the bulk modulus of the equivalent particle is the same as that obtained using the composite sphere model, when the interface moduli are calculated using Eq. (7). Therefore, the detailed procedures are not shown here. In order to obtain the shear moduli of the equivalent particles, we choose the remote strain (Fig. 1(a)) as

$$\varepsilon_{xx}^0 = \varepsilon_{yy}^0 = -\varepsilon_0, \quad \varepsilon_{zz}^0 = 2\varepsilon_0 \tag{11}$$

where ε_0 is a constant strain. Then the energy changes in Eqs. (4), (8) and (10) for the LSM, ISM and the interphase model can be expressed in a unified expression as

$$\Delta U_{\text{intf}} = -48\pi C_1 \varepsilon_0 \mu_1 (1 - \nu_1) R_{\text{I}}^3 \tag{12}$$

where C_1 is a constant to be determined later, and μ_1 and ν_1 are the shear modulus and Poisson ratio of the matrix, respectively. The value of C_1 depends on the chosen particular interface effect. Under the boundary conditions in Eq. (11), ΔU_{eq} in Eq. (1) can be expressed as

$$\Delta U_{\text{eq}} = V_{\text{eq}} \frac{90\varepsilon_0^2 \mu_1 (\mu_{\text{eq}} - \mu_1)(1 - \nu_1)}{\mu_1(7 - 5\nu_1) + 2\mu_{\text{eq}}(4 - 5\nu_1)} \tag{13}$$

where μ_{eq} and V_{eq} are the shear modulus and volume of the equivalent particle, respectively. The procedure for the solution of the constant C_1 for the three interface effects is as follows. Under the deviatoric homogeneous remote strain in Eq. (11), the general expressions for the displacements in an infinite region containing a spherical inhomogeneity with any of the above three interface effects are given by (Lur'e, 1964), in the spherical coordinates (r, θ, φ),

$$u_r = \left[12\nu A h^2 + 2B + \frac{2(5 - 4\nu)}{h^3} C - \frac{3D}{h^5}\right] r P_2(\cos\theta) \tag{14}$$

$$u_\theta = \left[(7 - 4\nu) A h^2 + B + \frac{2(1 - 2\nu)}{h^3} C + \frac{D}{h^5}\right] r \frac{\mathrm{d}P_2(\cos\theta)}{\mathrm{d}\theta} \tag{15}$$

where $P_2(\cos\theta)$ is the Legendre polynomial of order two, and $h = r/R_{\text{I}}$. It should be noted that the expressions in (14) and (15) are applicable to the spherical particle and the matrix material when we consider the composite with the linear-spring interface model or the interface stress model, whereas they are applicable to the spherical particle, the interphase and the matrix when we consider the composite with the interphase model. Therefore, the constants A, B, C and D are different for the three kinds of composite with the three interface effects. These constants are determined for each of the three interface conditions in Eqs. (2), (5) and (9), respectively, along with the remote boundary conditions and the condition to avoid singularity at the origin. For the particle, $C = D = 0$, and the remaining A and B are denoted by A_{I} and B_{I}. The constants for the matrix are denoted by A_1, B_1, C_1 and D_1, with A_1 and B_1 determined by the remote boundary conditions. For the interphase, the constants are represented by A_{c}, B_{c}, C_{c} and D_{c}. Therefore, for the LSM, there are four constants, A_{I}, B_{I} (in the particle), C_1 and D_1 (in the matrix) to be determined by Eq. (2); for the ISM, there are four constants, A_{I}, B_{I} (in the particle), C_1 and D_1 (in the matrix) to be determined by Eq. (5); and for the interphase model, there are eight constants, A_{I} and B_{I} (in the particle) C_1 and D_1 (in the matrix), and A_{c}, B_{c}, C_{c} and D_{c} in the interphase to be determined by Eq. (9).

After solving the boundary-value problem following the above procedure, the constant C_1 in Eq. (12) can be obtained. According to the energy equivalency condition $\Delta U_{\text{intf}} = \Delta U_{\text{eq}}$, the moduli κ_{eq} and μ_{eq} of the equivalent particle with the linear-spring interface effect are, with $\Delta U_{\text{intf}}^{\text{LSM}}$ given in Eq. (12) and ΔU_{eq} in Eq. (13),

$$\kappa_{\text{eq}} = \frac{m_r \kappa_{\text{I}} \mu_1}{3\kappa_{\text{I}} + m_r \mu_1} \tag{16}$$

$$\mu_{\text{eq}} = \mu_{\text{I}} \frac{24 M m_\theta + m_r(16M + m_\theta N)}{80 g_3 M + 4 g_3 m_\theta [10(7 - \nu_{\text{I}}) + M] + m_r[2 g_3(140 - 80\nu_{\text{I}} + 3M) + m_\theta N]} \tag{17}$$

where $M = g_3(7 + 5\nu_I)$, $N = 5(28 - 40\nu_I + M)$, and $g_3 = \mu_I/\mu_1$. κ_I, μ_I and ν_I are the bulk modulus, shear modulus and Poisson ratio of the particle, respectively. The two non-dimensional parameters m_r and m_θ are defined as $m_r = \alpha_n R_I/\mu_1$ and $m_\theta = \alpha_s R_I/\mu_1$.

The moduli of the equivalent particle with the interface stress effect are

$$\kappa_{eq} = \kappa_I + \frac{2\kappa^r \mu_1}{3} \tag{18}$$

$$\mu_{eq} = \mu_1 \frac{P}{2N + 8(7 - 10\nu_I)(3\kappa^r + \mu^r)} \tag{19}$$

in which

$$P = 2g_3 N + 4[84 + 5g_3(7 - \nu_I) - 120\nu_I]\mu^r + [5g_3(35 - 47\nu_I) + 4(7 - 10\nu_I)(1 + 5\mu^r)]\kappa^r \tag{20}$$

where κ^r and μ^r are two non-dimensional parameters, $\kappa^r = \kappa_s/(R_I\mu_1)$, $\mu^r = \mu_s/(R_I\mu_1)$, and $\kappa_s = 2(\mu_s + \lambda_s)$.

The bulk modulus of the equivalent particle with the interphase model is

$$\kappa_{eq} = \frac{4(1 - V_I)\kappa_c\mu_c + \kappa_I(3\kappa_c + 4V_I\mu_c)}{3(1 - V_I)\kappa_I + 3V_I\kappa_c + 4\mu_c} \tag{21}$$

where $V_I = [R_I/(R_I + t)]^3$, and κ_c and μ_c are the bulk and shear moduli of the interphase, respectively. The shear modulus of the equivalent particle with the interphase model is

$$\mu_{eq} = \mu_1 \frac{5 - 2V_I W_1(7 - 5\nu_1)}{5 + 4V_I W_1(4 - 5\nu_1)} \tag{22}$$

where $W_1 = C_1/\varepsilon_0$. As C_1 is proportional to ε_0, W_1 will be independent of ε_0. However, the expression of W_1 is not given here for its lengthiness.

3.3. Moduli of equivalent homogeneous fibres

Using the same procedure as for the spherical particles with the three interface effects, in this section, we will give the moduli of the equivalent homogeneous fibres for the fibre-reinforced composites with the interface effects. However, a cylindrical fibre with one of the interface effects will be replaced with an equivalent homogeneous transversely isotropic fibre, which should have five elastic constants, e.g. the longitudinal modulus E_{Leq}, the longitudinal Poisson ratio ν_{Leq}, the longitudinal shear modulus μ_{Leq}, the transverse plane-strain bulk modulus k_{eq}, and the transverse shear modulus μ_{Teq} (cf. Christensen, 1979). Here and in the following, the subscript "L" denotes a longitudinal property along the axis of a fibre, and "T" a transverse property perpendicular to it. For the three kinds of interface effect, E_{Leq}, ν_{Leq}, μ_{Leq} and k_{eq} of the equivalent fibres obtained by the present energy equivalency condition are the same as those obtained by the composite cylinder model of Hashin (1990) for the LSM, and Qiu and Weng (1991) for the interphase model. Therefore, the detailed procedures are not shown here. In order to obtain the transverse shear modulus of the equivalent fibre with one of the interface effects, we choose the remote strain as (Fig. 1(a))

$$\varepsilon^0_{xx} = \varepsilon_0, \quad \varepsilon^0_{yy} = -\varepsilon_0 \tag{23}$$

where we have assumed that the fibre is aligned with the z-axis in the Cartesian coordinate system. Then the energy changes in Eqs. (4), (8) and (10) for the LSM, ISM and the interphase model can be expressed in a unified expression as

$$\Delta U_{intf} = -8\pi c_1 \varepsilon_0 \mu_1 (1 - \nu_1)\rho_I^2 \tag{24}$$

where c_1 is a constant that is to be determined from the chosen interface effect, and ρ_I is the radius of the fibre. Under the boundary conditions in Eq. (23), ΔU_{eq} in Eq. (1) can be expressed as

$$\Delta U_{eq} = S_{eq} \frac{8\varepsilon_0^2 \mu_1(\mu_{Teq} - \mu_1)(1 - \nu_1)}{\mu_1 + \mu_{Teq}(3 - 4\nu_1)} \tag{25}$$

where S_{eq} is the area of the cross section of the equivalent fibre. The value of c_1 in Eq. (24) is determined in the way similar to that for the spherical particle. The corresponding elastic fields in the inhomogeneity, the interphase and the matrix can be found in the paper of Huang et al. (1994). Thus, for brevity, we do not reproduce the solution here. Instead, we only give the final expressions of the moduli of the equivalent fibre. In the following, we take a fibre as a transversely isotropic medium which has five elastic constants: plane-strain bulk modulus k_I, transverse shear modulus μ_{TI}, longitudinal shear modulus μ_{LI}, longitudinal modulus E_{LI}, and longitudinal Poisson ratio ν_{LI}. The matrix is assumed to be isotropic. The interface constitutive relations between the fibre and the matrix for the ISM and LSM are expressed in Eqs. (2) and (5), respectively, and the interphase between the fibre and the matrix is isotropic.

The five elastic constants of the equivalent fibre with the linear-spring interface effect are

$$k_{\mathrm{eq}}=\frac{m_\rho k_{\mathrm{I}}\mu_1}{2k_{\mathrm{I}}+m_\rho\mu_1} \tag{26}$$

$$\mu_{\mathrm{Teq}}=\mu_{\mathrm{TI}}\frac{3g_2(m_\rho+m_\phi)+m_\rho m_\phi(3+g_2-4v_{\mathrm{TI}})}{12g_2^2+g_2(m_\rho+m_\phi)(6+g_2-4v_{\mathrm{TI}})+m_\rho m_\phi(3+g_2-4v_{\mathrm{TI}})} \tag{27}$$

$$\mu_{\mathrm{Leq}}=\frac{m_z\mu_{\mathrm{LI}}\mu_1}{m_z\mu_1+\mu_{\mathrm{LI}}} \tag{28}$$

$$v_{\mathrm{Leq}}=v_{\mathrm{LI}} \tag{29}$$

$$E_{\mathrm{Leq}}=E_{\mathrm{LI}} \tag{30}$$

where $g_2=\mu_{\mathrm{TI}}/\mu_1$, and the three non-dimensional parameters m_ρ, m_ϕ and m_z are defined by $m_\rho=\alpha_n\rho_{\mathrm{I}}/\mu_1$, $m_\phi=\alpha_s\rho_{\mathrm{I}}/\mu_1$ and $m_z=\alpha_t\rho_{\mathrm{I}}/\mu_1$. v_{TI} is the transverse Poisson ratio of the fibre.

The five elastic constants of the equivalent fibre with the interface stress effect are

$$k_{\mathrm{eq}}=k_{\mathrm{I}}+\frac{\chi^r\mu_1}{4} \tag{31}$$

$$\mu_{\mathrm{Teq}}=\mu_1\frac{8g_2^2+(3-4v_{\mathrm{TI}})\chi^r+2g_2[12+5\chi^r-2v_{\mathrm{TI}}(8+3\chi^r)]}{8g_2+(3-4v_{\mathrm{TI}})(8+3\chi^r)} \tag{32}$$

$$\mu_{\mathrm{Leq}}=\mu_{\mathrm{LI}}+\mu^r\mu_1 \tag{33}$$

$$v_{\mathrm{Leq}}=\frac{2k_{\mathrm{I}}v_{\mathrm{LI}}+\lambda^r\mu_1}{2k_{\mathrm{I}}+(\lambda^r+2\mu^r)\mu_1} \tag{34}$$

$$E_{\mathrm{Leq}}=E_{\mathrm{LI}}+\frac{4k_{\mathrm{I}}\mu_1[2(1+v_{\mathrm{LI}}^2)\mu^r+(1-v_{\mathrm{LI}})^2\lambda^r]}{2k_{\mathrm{I}}+(\lambda^r+2\mu^r)\mu_1} \tag{35}$$

where $\chi^r=4\mu^r+2\lambda^r$, $\mu^r=\mu_s/(\rho_{\mathrm{I}}\mu_1)$ and $\lambda^r=\lambda_s/(\rho_{\mathrm{I}}\mu_1)$.

The moduli of the equivalent fibre with the interphase model are

$$k_{\mathrm{eq}}=\frac{(1-V_{\mathrm{I}})k_c\mu_c+k_{\mathrm{I}}(k_c+V_{\mathrm{I}}\mu_c)}{(1-V_{\mathrm{I}})k_{\mathrm{I}}+V_{\mathrm{I}}k_c+\mu_c} \tag{36}$$

$$\mu_{\mathrm{Teq}}=\mu_1\frac{1-V_{\mathrm{I}}w_1}{1+V_{\mathrm{I}}w_1(3-4v_1)} \tag{37}$$

$$\mu_{\mathrm{Leq}}=\mu_c+\frac{2V_{\mathrm{I}}\mu_c(\mu_{\mathrm{LI}}-\mu_c)}{(1-V_{\mathrm{I}})\mu_{\mathrm{LI}}+(1+V_{\mathrm{I}})\mu_c} \tag{38}$$

$$v_{\mathrm{Leq}}=V_{\mathrm{I}}v_{\mathrm{LI}}+(1-V_{\mathrm{I}})v_c+\frac{V_{\mathrm{I}}\mu_c(1-V_{\mathrm{I}})(k_{\mathrm{I}}-k_c)(v_{\mathrm{LI}}-v_c)}{(1-V_{\mathrm{I}})k_c\mu_c+k_{\mathrm{I}}(k_c+V_{\mathrm{I}}\mu_c)} \tag{39}$$

$$E_{\mathrm{Leq}}=V_{\mathrm{I}}E_{\mathrm{LI}}+(1-V_{\mathrm{I}})E_c+\frac{4V_{\mathrm{I}}(1-V_{\mathrm{I}})(v_{\mathrm{LI}}-v_c)^2}{\dfrac{1-V_{\mathrm{I}}}{k_{\mathrm{I}}}+\dfrac{V_{\mathrm{I}}}{k_c}+\dfrac{1}{\mu_c}} \tag{40}$$

where $V_{\mathrm{I}}=[\rho_{\mathrm{I}}/(\rho_{\mathrm{I}}+t)]^2$, and $w_1=c_1/\varepsilon_0$. As c_1 is proportional to ε_0, w_1 will be independent of ε_0. However, the expression of w_1 is not given here for its lengthiness.

4. Energy framework and equivalent inclusion method

4.1. Energy framework

Having replaced the spherical particles/fibres with the interface effects by equivalent homogeneous particles/fibres which are perfectly bonded to the corresponding matrix materials, we can use various micromechanical schemes to predict the effective moduli of two- and multi-phase composites with these interface effects. There are many micromechanical schemes in the literature, e.g. the generalized self-consistent method (GSCM, Christensen and Lo, 1979), the Mori–Tanaka method (MTM, Mori and Tanaka, 1973; Benveniste, 1987) and the double-inclusion model (Hori and Nemat-Nasser, 1993), etc. For a comprehensive exposition, one can refer to the monographs of Aboudi (1991), Nemat-Nasser and Hori (1999), and Torquato (2002). It is noted that Tan et al. (2005a) predicted the effective stress–strain relations of composites containing spherical particles with the piecewise linear interface cohesive law using the Mori–Tanaka method. In their prediction, the Mori–Tanaka method is modified to incorporate the displacement discontinuity and the interface law at the particle/matrix interface. In this paper, we shall use a micromechanical scheme that was recently proposed by Duan et al. (in press) along with the above replacement procedure to predict the effective moduli of the composites with the interface effects. It has been shown that the distinguished feature of the micromechanical scheme of Duan et al. (in press) is that, whilst its predictions are almost identical to the classical generalized self-consistent method (GSCM, Christensen and Lo, 1979), and the third-order approximation (TOA, Torquato, 1998), the expressions for the effective moduli have very simple closed forms. For the sake of completeness, we begin with the energy equivalency framework of Hill (1963).

Hill (1963) established the energy equivalency framework for composites. Huang and Hwang (1995) generalized this framework to anisotropic matrices and inhomogeneities, and applied it to the dilute approximation, the self-consistent method, the generalized self-consistent method, and the Mori–Tanaka method. Dong et al. (2005) generalized the theoretical framework of Huang and Hwang (1995) to multiple transversely isotropic fibres and transversely isotropic matrices. Following Hill (1963), and Huang and Hwang (1995), consider a representative volume element (RVE) of a multiphase (N-phase) composite consisting of a continuous matrix and $N-1$ kinds of discrete inhomogeneity. The corresponding stiffness tensors of the inhomogeneities are $\mathbf{C}_I\,(I=2,\ldots,N)$, and that of the matrix is $\mathbf{C}_1$. Applying a homogeneous traction boundary conditions $\mathbf{\Sigma}(S)=\boldsymbol{\sigma}^0\cdot\mathbf{N}$ on the external surface S of the RVE, where $\boldsymbol{\sigma}^0$ is the uniform stress tensor when the material is homogeneous and $\mathbf{N}$ is the exterior unit normal vector to S, then the strain energy U_{macro} of the composite material is given by

$$U_{\text{macro}}=\frac{1}{2}\boldsymbol{\sigma}^0:\overline{\mathbf{C}}^{-1}:\boldsymbol{\sigma}^0V \tag{41}$$

where $\overline{\mathbf{C}}$ is the effective stiffness tensor of the composite, and V is the volume of it. The strain energy of the composite is also the sum of the energy in the inhomogeneities and the matrix

$$U_{\text{micro}}=\frac{1}{2}\boldsymbol{\sigma}^0:\left[\mathbf{C}_1^{-1}:\boldsymbol{\sigma}^0+\sum_{I=2}^{N}f_I\left(\mathbf{C}_I^{-1}-\mathbf{C}_1^{-1}\right):\bar{\boldsymbol{\sigma}}^I\right]V \tag{42}$$

where f_I is the volume fraction of the I-th kind of inhomogeneity. According to the energy equivalence $U_{\text{micro}}=U_{\text{macro}}$, the following equation can be obtained (Hill, 1963):

$$\overline{\mathbf{C}}^{-1}=\mathbf{C}_1^{-1}+\sum_{I=2}^{N}f_I(\mathbf{C}_I^{-1}-\mathbf{C}_1^{-1}):\overline{\mathbf{T}}^I \tag{43}$$

Likewise, applying a homogeneous strain boundary conditions $\mathbf{u}(S)=\boldsymbol{\varepsilon}^0\cdot\mathbf{x}$ on the external surface S, the following equation can be obtained (Hill, 1963):

$$\overline{\mathbf{C}}=\mathbf{C}_1+\sum_{I=2}^{N}f_I(\mathbf{C}_I-\mathbf{C}_1):\overline{\mathbf{E}}^I \tag{44}$$

$\overline{\mathbf{T}}^I$ in Eq. (43) and $\overline{\mathbf{E}}^I$ in Eq. (44) are the stress and strain concentration tensors in the Ith inhomogeneity, namely,

$$\bar{\boldsymbol{\sigma}}^I=\overline{\mathbf{T}}^I:\boldsymbol{\sigma}^0,\quad \bar{\boldsymbol{\varepsilon}}^I=\overline{\mathbf{E}}^I:\boldsymbol{\varepsilon}^0 \tag{45}$$

in which $\bar{\boldsymbol{\varepsilon}}^I$ and $\bar{\boldsymbol{\sigma}}^I$ are the volume average strain and stress tensors in the Ith inhomogeneity, respectively.

4.2. GSCM for two-phase composites

It should be emphasized that Eqs. (43) and (44) are exact representations of the effective moduli. The approximation nature of various micromechanical schemes comes from the evaluation of the average strains and stresses in the inhomogeneities and the matrix. Many micromechanical schemes can be used to evaluate $\overline{\mathbf{T}}^I$ and $\overline{\mathbf{E}}^I$ thus to give various predictions of the effective moduli. For linear composites containing non-overlapping identical spheres, Segurado and LLorca (2002) conducted detailed numerical computation of the effective moduli and compared their results with three analytical models, namely, the Mori–Tanaka method (MTM, Mori and Tanaka, 1973, Benveniste, 1987), the generalized self-consistent method (GSCM, Christensen and Lo, 1979), and Torquato's third-order approximation (TOA, Torquato, 1998). Following the comparisons of Segurado and LLorca (2002), and the studies of Ma et al. (2004), it appears that from an overall point of view, the GSCM and the TOA tend to give the best results for spherical particle-reinforced composites.

The GSCM evaluates $\overline{\mathbf{E}}^I$ or $\overline{\mathbf{T}}^I$ based on the three-phase model where an inhomogeneity is embedded in a finite matrix shell that, in turn, is embedded in an infinite equivalent medium with the yet-unknown effective properties of the composite, as shown in Fig. 2(a). The outer radius R_{m} (or ρ_{m}) of the spherical (or circular) matrix shell is

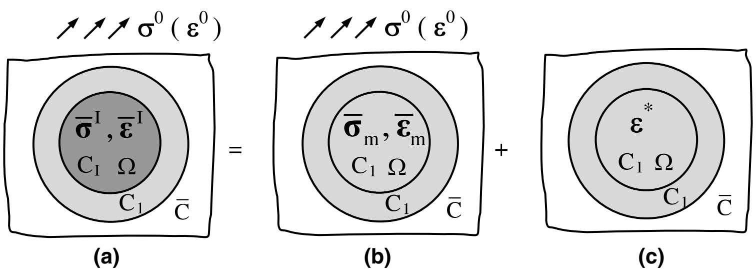

Fig. 2. The GSCM (three-phase) configuration for a composite containing spherical (circular) inhomogeneities (a). The Eshelby equivalent inclusion method in a volume average sense for the three-phase configuration ((b) and (c)).

related to the radius R_{I} (or ρ_{I}) of the spherical (or circular) inhomogeneity through the volume fraction $f_{\mathrm{I}} = R_{\mathrm{I}}^3/R_{\mathrm{m}}^3$ ($f_{\mathrm{I}} = \rho_{\mathrm{I}}^2/\rho_{\mathrm{m}}^2$ for circular inhomogeneity). The GSCM has emphasized the importance of the matrix atmosphere. Zheng and Du (2001) have also emphasized this and proposed an effective self-consistent method (ESCM) which is also based on a three-phase model.

For a two-phase composite, the effective moduli predicted by the GSCM can be easily obtained by substituting the strain concentration tensor $\overline{\mathbf{E}}^I$ into Eq. (44). $\overline{\mathbf{E}}^I$ can be calculated in terms of the configuration shown in Fig. 2(a) using the procedure of Christensen and Lo (1979). While the effective bulk modulus is given by a simple formula, the predicted effective shear modulus needs to be calculated from a quadratic equation with lengthy coefficients. Recently, Duan et al. (in press) proposed a new micromechanical scheme. In the scheme of Duan et al. (in press), the strain concentration tensor $\overline{\mathbf{E}}^I$ is not directly calculated using the configuration in Fig. 2(a). Instead, it is calculated using the Eshelby equivalent inclusion method in a volume average sense shown in Fig. 2(b) and (c). This method to calculate the strain concentration tensor is briefly described below.

Assume that the volume average stress in the inhomogeneity Ω in the three-phase configuration in Fig. 2(a) is $\bar{\boldsymbol{\sigma}}^I$ while the remote stress is $\boldsymbol{\sigma}^0$. For the same remote stress, when we replace the spherical inhomogeneity with the stiffness tensor $\mathbf{C}_{\mathrm{I}}$ by the matrix material with the stiffness tensor $\mathbf{C}_1$, the volume average stress in the same region Ω is denoted by $\bar{\boldsymbol{\sigma}}_{\mathrm{m}}$, as shown in Fig. 2(b). This volume average stress $\bar{\boldsymbol{\sigma}}_{\mathrm{m}}$ can be related to the remote stress by the relation $\bar{\boldsymbol{\sigma}}_{\mathrm{m}} = \mathbf{B} : \boldsymbol{\sigma}^0$, where the fourth-order tensor $\mathbf{B}$ is equal to the classical stress concentration tensor $\mathbf{T}^0$ (Duan et al., in press). Generally, $\bar{\boldsymbol{\sigma}}_{\mathrm{m}}$ is different from $\bar{\boldsymbol{\sigma}}^I$. As in the classical Eshelby equivalent inclusion method, the spherical matrix region Ω is further given a uniform eigenstrain $\boldsymbol{\varepsilon}^*$ (Fig. 2(c)) such that the following equivalency condition is satisfied:

$$\mathbf{C}_{\mathrm{I}} : (\bar{\boldsymbol{\varepsilon}}_{\mathrm{m}} + \bar{\boldsymbol{\varepsilon}}') = \mathbf{C}_1 : (\bar{\boldsymbol{\varepsilon}}_{\mathrm{m}} + \bar{\boldsymbol{\varepsilon}}' - \boldsymbol{\varepsilon}^*) \tag{46}$$

where a bar denotes the volume average. The disturbed strain $\bar{\boldsymbol{\varepsilon}}'$ is related to the interior Eshelby tensor $\overline{\mathbf{S}}^I$ through

$$\bar{\boldsymbol{\varepsilon}}' = \overline{\mathbf{S}}^I : \boldsymbol{\varepsilon}^* \tag{47}$$

Following the classical Eshelby equivalent inclusion method in a volume average sense for the three-phase configuration (Duan et al., in press), the approximate volume average stress concentration tensor $\overline{\mathbf{T}}^*$ that relates the volume average stress $\bar{\boldsymbol{\sigma}}^I$ to the remote stress $\boldsymbol{\sigma}^0$ through the relation $\bar{\boldsymbol{\sigma}}^I = \overline{\mathbf{T}}^* : \boldsymbol{\sigma}^0$ can be expressed as follows:

$$\overline{\mathbf{T}}^* = [\mathbf{I}^{(4s)} - \mathbf{C}_I : \overline{\mathbf{S}}^I : (\mathbf{C}_I^{-1} - \mathbf{C}_1^{-1})]^{-1} : \mathbf{C}_I : \mathbf{C}_1^{-1} : \mathbf{B} \tag{48}$$

where $\mathbf{I}^{(4s)}$ is the fourth-order symmetric identity tensor in three-dimensional space (Nemat-Nasser and Hori, 1999), $\overline{\mathbf{S}}^I$ is the volume average Eshelby tensor for the spherical region Ω in Fig. 2(c), which has been given in the paper of Duan et al. (in press). For a spherical isotropic particle in an isotropic matrix, the stress concentration tensor in Eq. (48) can be expressed as

$$\overline{\mathbf{T}}^* = \alpha^* \mathbf{J}_3 + \beta^* \mathbf{K}_3 \tag{49}$$

in which

$$\mathbf{J}_3 = \frac{1}{3}\mathbf{I}^{(2)} \otimes \mathbf{I}^{(2)}, \quad \mathbf{K}_3 = -\frac{1}{3}\mathbf{I}^{(2)} \otimes \mathbf{I}^{(2)} + \mathbf{I}^{(4s)} \tag{50}$$

where $\mathbf{I}^{(2)}$ is the second-order identity tensor in three-dimensional space. Likewise, the strain concentration tensor $\overline{\mathbf{E}}^*$, which relates the volume average strain $\bar{\boldsymbol{\varepsilon}}^I$ to the remote strain $\boldsymbol{\varepsilon}^0$ in the relation $\bar{\boldsymbol{\varepsilon}}^I = \overline{\mathbf{E}}^* : \boldsymbol{\varepsilon}^0$, is given as

$$\overline{\mathbf{E}}^* = [\mathbf{I}^{(4s)} - \overline{\mathbf{S}}^I : \mathbf{C}_1^{-1} : (\mathbf{C}_1 - \mathbf{C}_I)]^{-1} : \mathbf{A} \tag{51}$$

where the fourth-order tensor $\mathbf{A}$ relates the volume average strain $\bar{\boldsymbol{\varepsilon}}_{\mathrm{m}}$ to the remote strain $\boldsymbol{\varepsilon}^0$ through the relation $\bar{\boldsymbol{\varepsilon}}_{\mathrm{m}} = \mathbf{A} : \boldsymbol{\varepsilon}^0$ (Fig. 2(b)), and $\mathbf{A} = \mathbf{C}_I^{-1} : \mathbf{B} : \mathbf{C}_1$.

It is found that the dilatational component α^* of the approximate average stress concentration tensor $\overline{\mathbf{T}}^*$ in Eq. (49) is identical to that of the exact average stress concentration tensors $\overline{\mathbf{T}}^I$ calculated directly by solving the boundary-value problem in Fig. 2(a), and the deviatoric component β^* has practically the same numerical values as those of the exact counterpart for composites containing spherical particles of various stiffnesses (Duan et al., in press). Therefore, the approximate stress concentration tensor $\overline{\mathbf{T}}^*$ obtained using the Eshelby equivalent inclusion method in the above volume average sense is very accurate. Thus we shall replace $\overline{\mathbf{T}}^I$ in the general expression (43) with $\overline{\mathbf{T}}^*$ to predict the effective compliance tensor of composites containing randomly distributed spherical inhomogeneities. Duan et al. (in press) also found that the effective bulk and shear moduli obtained by substituting the stress

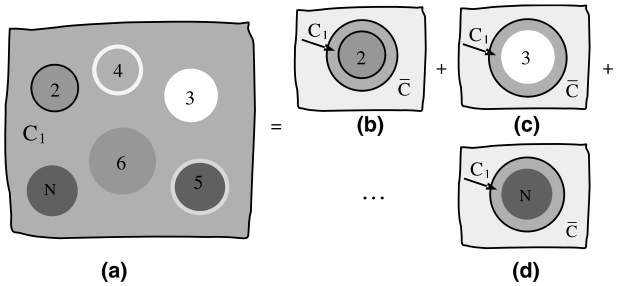

Fig. 3. A scheme showing how to decompose a multiphase composite into multiple composites to calculate the stress (strain) concentration tensors. A composite with multiple inhomogeneities (a); 2nd sub-composite (b); 3rd sub-composite (c); and Nth sub-composite (d).

concentration tensor $\overline{\mathbf{T}}^*$ in Eq. (49) into Eq. (43) are identical to those obtained by substituting the strain concentration tensor $\overline{\mathbf{E}}^*$ in Eq. (51) into Eq. (44), which means that this method is self-consistent indeed. Thus, either Eq. (43) or (44) can be used to predict the effective moduli.

The above Eshelby equivalent inclusion method in a volume average sense is also applicable to the circular inhomogeneity, and $\overline{\mathbf{S}}^{\mathrm{I}}$, $\overline{\mathbf{T}}^I$ and $\overline{\mathbf{T}}^*$ for the circular inhomogeneity have the similar properties to those of the spherical inhomogeneity. $\overline{\mathbf{S}}^I$ for the circular inhomogeneity in the plane-strain state is given below

$$\overline{\mathbf{S}}^{\mathrm{I}} = \xi_{\mathrm{I}}\mathbf{J_2} + \varsigma_{\mathrm{I}}\mathbf{K_2} \tag{52}$$

where

$$\mathbf{J}_2 = \frac{1}{2}\mathbf{I}'^{(2)} \otimes \mathbf{I}'^{(2)}, \quad \mathbf{K}_2 = -\frac{1}{2}\mathbf{I}'^{(2)} \otimes \mathbf{I}'(2) + \mathbf{I}'^{(4s)} \tag{53}$$

$$\xi_{\mathrm{I}} = 1 - \frac{4}{N_1}(1-2\nu_1)[1-\lambda^2 + (1+\lambda^2-2\nu_1)g_I] \tag{54}$$

$$\varsigma_{\mathrm{I}} = \frac{3-4\nu_1}{4(1-\nu_1)} - \frac{2\lambda^2}{N_2}\left[3\lambda^2(1-\lambda^2)(1-g_I) + \frac{H_{12}}{(3+g_{\mathrm{I}}-4\bar{\nu})}\right] \tag{55}$$

in which

$$\begin{aligned} N_1 &= 8(1-\nu_1)[1+g_I(1-2\nu_1)] \\ N_2 &= 8(1-\nu_1)[1+g_I(3-4\nu_1)] \\ H_{12} &= g_I^2[3(4-\lambda^2) - 24\nu_1 + 16\nu_1^2] \\ &\quad - 2g_I(3\lambda^2 - 4\nu_1)(1-2\bar{\nu}) \\ &\quad - (4-3\lambda^2)(3-4\bar{\nu}) \end{aligned} \tag{56}$$

where $\lambda = \rho_{\mathrm{I}}/\rho_m$, and $g_I = \bar{\mu}/\mu_1$. $\mathbf{I}'^{(2)}$ and $\mathbf{I}'^{(4s)}$ are the second-order identity tensor and the fourth-order symmetric identity tensor in two-dimensional space (Nemat-Nasser and Hori, 1999), respectively.

4.3. GSCM for multiphase composites

Eqs. (43) and (44), together with the average stress and strain concentration tensors can be used to calculate the effective bulk and shear moduli of multiphase composites. Fig. 3 shows how to approximately decompose a multiphase composite into multiple composites each of which contains only one kind of inhomogeneity, and constitutes a generalized self-consistent three-phase model as shown in Fig. 2(a) for the concerned inhomogeneity. For each of the multiple composites, the stress (strain) concentration tensor $\overline{\mathbf{T}}^*(\overline{\mathbf{E}}^*)$ is calculated using the expression in Eqs. (48) and (51), following the procedure shown in Fig. 2. Then the effective moduli of the multiphase composite are calculated from Eq. (43) (Eq. (44)) by substituting the obtained stress (strain) concentration tensors and other parameters into it.

In general, Eqs. (43) and (48) or Eqs. (44) and (51) constitute the basic equations to obtain the effective moduli of the multiphase composites. These are nonlinear coupled algebraic equations and have to be solved numerically. However, as will be shown in Part II, instead of solving these nonlinear coupled equations numerically, we can calculate the effective moduli using an alternative simple decoupled method proposed by Huang et al. (1994). It will be seen that this simple method gives very accurate results for various composites.

5. Conclusions

In this part of the two-part paper, a unified micromechanical framework is presented to predict the effective moduli of particle- or fibre-reinforced composites with interface effects. This framework comprises a replacement procedure and the generalized self-consistent prediction of the effective moduli. Both of these procedures are different from the conventional ones in that the elastic constants of the equivalent homogeneous particles/fibres are calculated based upon an energy equivalency condition, and the generalized self-consistent prediction is based upon the Eshelby equivalent inclusion method in an average sense for the three-phase configuration. As will be shown in Part II, this scheme gives simple expressions of the effective moduli of the composites with the interface effects.

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References

Aboudi, J., 1991. Mechanics of Composite Materials – A Unified Micromechanical Approach. Elsevier, Amsterdam.

Benveniste, Y., 1985. The effective mechanical behaviour of composite materials with imperfect contact between the constituents. Mech. Mater. 4, 197–208.

Benveniste, Y., 1987. A new approach to the application of Mori–Tanaka's theory in composite materials. Mech. Mater. 6, 147–157.

Christensen, R.M., 1979. Mechanics of Composite Materials. Wiley-Interscience Publication, New York.

Christensen, R.M., Lo, K.H., 1979. Solutions for effective shear properties in three phase sphere and cylinder models. J. Mech. Phys. Solids 27, 315–330.

Cuenot, S., Frétigny, C., Demoustier-Champagne, S., Nysten, B., 2004. Surface tension effect on the mechanical properties of nanomaterials measured by atomic force microscopy. Phys. Rev. B 69, 165410-1–165410-5.

Dingreville, R., Qu, J., Cherkaoui, M., 2005. Surface free energy and its effect on the elastic behaviour of nano-sized particles, wires and films. J. Mech. Phys. Solids 53, 1827–1854.

Dong, X.N., Zhang, X.H., Huang, Y.Y., Guo, X.E., 2005. A generalized self-consistent estimate for the effective elastic moduli of fiber-reinforced composite materials with multiple transversely isotropic inclusions. Int. J. Mech. Sci. 47, 922–940.

Duan, H.L., Wang, J., Huang, Z.P., Karihaloo, B.L., 2005a. Size-dependent effective elastic constants of solids containing nano-inhomogeneities with interface stress. J. Mech. Phys. Solids 53, 1574–1596.

Duan, H.L., Wang, J., Huang, Z.P., Karihaloo, B.L., 2005b. Eshelby formalism for nano-inhomogeneities. Proc. R. Soc. A 461, 3335–3353.

Duan, H.L., Wang, J., Huang, Z.P., Luo, Z.Y., 2005c. Stress concentration tensors of inhomogeneities with interface effects. Mech. Mater. 37, 723–736.

Duan, H.L., Wang, J., Huang, Z.P., Zhong, Y., 2005d. Stress fields of a spheroidal inhomogeneity with an interphase in an infinite medium under remote loadings. Proc. R. Soc. A 461, 1055–1080.

Duan, H.L., Jiao, Y., Yi, X., Huang, Z.P., Wang, J., in press. Solutions of inhomogeneity problems with graded shells and application to core-shell nanoparticles and composites. J. Mech. Phys. Solids.

Eshelby, J.D., 1957. The determination of the elastic field of an ellipsoidal inclusion and related problems. Proc. R. Soc. A 241, 376–396.

Garboczi, E.J., Berryman, J.G., 2001. Elastic moduli of a material containing composite inclusions: effective medium theory and finite element computations. Mech. Mater. 33, 455–470.

Gurtin, M.E., Murdoch, A.I., 1975. A continuum theory of elastic material surfaces. Arch. Ration. Mech. Anal. 57, 291–323.

Hashin, Z., 1990. Thermoelastic properties of fiber composites with imperfect interface. Mech. Mater. 8, 333–348.

Hashin, Z., 1991. Thermoelastic properties of particulate composites with imperfect interface. J. Mech. Phys. Solids 39, 745–762.

Hill, R., 1963. Elastic properties of reinforced solids: some theoretical principles. J. Mech. Phys. Solids 11, 357–372.

Hori, M., Nemat-Nasser, S., 1993. Double-inclusion model and overall moduli of multi-phase composites. Mech. Mater. 14, 189–206.

Huang, Y., Hwang, K.C., 1995. A unified energy approach to a class of micromechanics models for microcracked solids. Acta Mech. Solida Sinica 8, 110–120.

Huang, Z.P., Wang, J., in press. A theory of hyperelasticity of multiphase media with interface energy effect. Acta. Mech.

Huang, Y., Hu, K.X., Wei, X., Chandra, A., 1994. A generalized self-consistent mechanics method for composite materials with multiphase inclusions. J. Mech. Phys. Solids 42, 491–504.

Jiang, B., Weng, G.J., 2004. A generalized self-consistent polycrystal model for the yield strength of nanocrystalline materials. J. Mech. Phys. Solids 52, 1125–1149.

Karihaloo, B.L., Viswanathan, K., 1988a. A partially debonded ellipsoidal inclusion in an elastic medium Part I. Stress and displacement fields. Mech. Mater. 7, 191–197.

Karihaloo, B.L., Viswanathan, K., 1988b. A partially debonded ellipsoidal inclusion in an elastic medium. Part II. Stress intensity factors and debond opening displacement. Mech. Mater. 7, 199–203.

Lur'e, A.I., 1964. Three-dimensional Problems of Theory of Elasticity. Interscience, New York.

Ma, H., Hu, G., Huang, Z.P., 2004. A micromechanical method for particulate composites with finite particle concentration. Mech. Mater. 36, 359–368.

Mori, T., Tanaka, K., 1973. Average stress in matrix and average elastic energy of materials with misfitting inclusions. Acta Metall. 21, 571–574.

Müller, P., Saúl, A., 2004. Elastic effects on surface physics. Surf. Sci. Rep. 54, 157–258.

Mura, T., Furuhashi, R., 1984. The elastic inclusion with a sliding interface. J. Appl. Mech. 51, 308–310.

Nemat-Nasser, S., Hori, M., 1999. Micromechanics: Overall Properties of Heterogeneous Materials, second ed. Elsevier, Amsterdam.

Nix, W.D., Gao, H.J., 1998. An atomistic interpretation of interface stress. Scripta Mater. 39, 1653–1661.

Ponte Castañeda, P., Suquet, P., 1998. Nonlinear composites. Adv. Appl. Mech. 34, 171–302.

Qiu, Y.P., Weng, G.J., 1991. Elastic moduli of thickly coated particle and fiber-reinforced composites. J. Appl. Mech. 58, 388–398.

Qu, J., 1993. The effect of slightly weakened interfaces on the overall elastic properties of composites. Mech. Mater. 14, 269–281.

Schiøtz, J., Di Tolla, F.D., Jacobsen, K.W., 1998. Softening of nanocrystalline metals at very small grain sizes. Nature 391, 561–563.

Segurado, J., LLorca, J., 2002. A numerical approximation to the elastic properties of sphere-reinforced composites. J. Mech. Phys. Solids 50, 2107–2121.

Shen, L.X., Li, J., 2005. Homogenization of a fibre/sphere with an inhomogeneous interphase for the effective elastic moduli of composites. Proc. R. Soc. A 461, 1475–1504.

Shenoy, V.B., 2005. Atomistic calculations of elastic properties of metallic fcc crystal surfaces. Phys. Rev. B 71, 094104-1–094104-11.

Shuttleworth, R., 1950. The surface tension of solids. Proc. Phys. Soc. A 63, 444–457.

Streitz, F.H., Cammarata, R.C., Sieradzki, K., 1994. Surface-stress effects on elastic properties. II: Metallic multilayers. Phys. Rev. B 49, 10707–10716.

Sun, L., Wu, Y.M., Huang, Z.P., Wang, J., 2004. Interface effect on the effective bulk modulus of a particle-reinforced composite. Acta Mech. Sinica 20, 676–679.

Tan, H., Huang, Y., Liu, C., Geubelle, P.H., 2005a. The Mori–Tanaka method for composite materials with nonlinear interface debonding. Int. J. Plasticity 21, 1890–1918.

Tan, H., Liu, C., Huang, Y., Geubelle, P.H., 2005b. The cohesive law for the particle/matrix interfaces in high explosives. J. Mech. Phys. Solids 53, 1892–1917.

Theocaris, P.S., 1987. The Mesophase Concept in Composites. Springer-Verlag, Berlin.

Torquato, S., 1998. Effective stiffness tensor of composite media. II: Applications to isotropic dispersions. J. Mech. Phys. Solids 46, 1411–1440.

Torquato, S., 2002. Random Heterogeneous Materials: Microstructure and Macroscopic Properties. Springer-Verlag, New York.

Walpole, L.J., 1978. A coated inclusion in an elastic medium. Math. Proc. Camb. Phil. Soc. 83, 495–506.

Wang, J., Duan, H.L., Zhang, Z., Huang, Z.P., 2005. An anti-interpenetration model and connections between interphase and interface models in particle-reinforced composites. Int. J. Mech. Sci. 47, 701–708.

Wei, Y.J., Anand, L., 2004. Grain-boundary sliding and separation in polycrystalline metals: application to nanocrystalline fcc metals. J. Mech. Phys. Solids 52, 2587–2616.

Zhang, T.-Y., Hack, J.E., 1992. On the elastic stiffness of grain boundaries. Phys. Status Solidi A 131, 437–443.

Zheng, Q.S., Du, D.X., 2001. An explicit and universally applicable estimate for the effective properties of multiphase composites which accounts for inclusion distribution. J. Mech. Phys. Solids 49, 2765–2788.

Zhong, Z., Meguid, S.A., 1997. On the elastic field of a spherical inhomogeneity with an imperfectly bonded interface. J. Elasticity 46, 91–113.

Zhong, Y., Wang, J., Wu, Y.M., Huang, Z.P., 2004. Effective moduli of particle-filled composite with inhomogeneous interphase. Part II: Mapping method and evaluation. Compos. Sci. Technol. 64, 1353–1362.