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Solids containing spherical nano-inclusions with interface stresses: Effective properties and thermal–mechanical connections

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Abstract

This work examines the overall thermoelastic behavior of solids containing spherical inclusions with surface effects. Elastic response is evaluated as a superposition of separate solutions for isotropic and deviatoric overall loads. Using a variational approach, we construct the Euler–Lagrange equation together with the natural transition (jump) conditions at the interface. The overall bulk modulus is derived in a simple form, based on the construction of neutral composite sphere. The transverse shear modulus estimate is derived using the generalized self-consistent method. Further, we show that there exists an exact connection between effective thermal expansion and bulk modulus. This connection is valid not only for a composite sphere, but also for a matrix-based composite reinforced by many randomly distributed spheres of the same size, and can be viewed as an analog of Levin's formula for composites with surface effects.

Keywords: Surface stress; Effective properties; Composites; Thermo-mechanical connections

1. Introduction

Surface stress in solids is defined as a configurational force that is work-conjugate to surface strain with respect to the free surface energy. A review of this subject was given by Cammarata (1994). Our objective in this work is to assess the overall thermoelastic behavior of solids containing spherical nano-inclusions with the surface stress effects. Elastic properties of both matrix, inclusions and inclusion surfaces are isotropic. Therefore, the overall or effective elastic response of the composite is also isotropic. This response is derived as a superposition of two separate solutions under isotropic and deviatoric overall strain states. We first derive the energy potential of the system incorporating the surface effects for each of the two deformation modes.

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Using variational approaches, we construct the Euler–Lagrange equations together with the interface jump conditions. The interface conditions are characterized by continuities of displacements across the interface, together with a jump condition in traction. The mathematical framework allows us to resolve the field solutions of the boundary value problems. As in the method of composite spheres assemblages (Hashin, 1962), or neutral inhomogeneities (Milton, 2002), a representative volume element of a composite sphere is adopted for determination of the overall bulk modulus in simple closed form. Under uniform overall deviatoric strain, we derive an estimate of the effective shear modulus by the generalized self-consistent method (Christensen and Lo, 1979). The critical part of deviatoric deformation is the derivation of the jump conditions in traction. The effective shear modulus is derived in the form of a quadratic algebraic equation.

Under a uniform temperature change, we prove an exact thermo-mechanical linkage. This connection is valid for a general composite medium containing many spheres of the same size. The spheres can be arbitrarily distributed in the matrix or arranged in a preferred manner. In particular, we show that a uniform strain field is created in the composite by application of a certain combination of external isotropic strain and uniform change in temperature, or piecewise uniform eigenstrains in the phases. Mechanical unloading to zero overall strain then reveals existence of an exact size-dependent connection that provides the effective thermal expansion coefficient as a simple function of the bulk modulus. This connection can be viewed as generalization of Levin's (1967) formula for the system with surface effects.

Related studies include Sharma et al. (2003) who employed the variational approach to derive the elastic field in a spherical inhomogeneity loaded by overall isotropic strain and uniform local eigenstrain. Yang (2004) derived the effective bulk and shear moduli of composites containing spherical nano-cavities at dilute concentrations, in which the surface effect is simply simulated by a constant residual tension. Sharma and Ganti (2004) derived closed-form expressions for the Eshelby tensor for spherical and cylindrical inclusions with surface effects. A recent study (Duan et al., 2005) generalized several micromechanical averaging procedures for estimating effective elastic moduli of composites by incorporating the surface/interface stress effect. The interface conditions associated with the bulk and shear deformations are directly extracted from a generalized Young–Laplace equation by Povstenko (1993). Here we start from the simple shear deformation, using a variational approach, the interface jump conditions were derived from the natural transition condition at the interface.

The plan of the paper is as follows. In Section 2, we derive the free energy of the system under the two overall uniform strain states. Section 3 shows that a uniform expansion field can be generated by application of certain magnitudes of uniform overall strain and temperature change. We construct an exact connection between the effective thermal expansion coefficient and the bulk modulus. The effective bulk and shear moduli are derived in Section 4. Numerical calculations in Section 5 illustrate the effect of surface stresses on local fields and overall moduli.

2. Interface conditions with surface effect

Two independent interface stresses have been reported in the literature: one is associated with coherent interface in which the tangential strains are equal on both sides of the phases, the other allows that different tangential strains may occur at the interface (Brooks, 1952). In the present study we are concerned with the former situation in which no atomic bonds are broken in the spherical interface. We will adopt the spherical coordinate system (r, θ, φ) in the formulation. Interface stresses and strains can be described as (2×2) symmetric tensors in the tangent plane (components normal to the surface are excluded). Development of the ideas underlying the concept of surface or interface stress in solids was pioneered by Shuttleworth (1950), Herring (1951), Gurtin and Murdoch (1975) and Cahn (1980). A more extensive treatment, allowing for displacement jumps and their gradients, with corresponding conjugate forces, was developed by Gurtin et al. (1998). Of interest here are coherent interfaces which preserve continuity of displacements and of the interior strain tensor components in the tangential plane. Under such circumstances, the surface stress tensor $\sigma^s_{\alpha\beta}$ is related to the deformation dependent surface energy $\mathscr{G}(\varepsilon_{\alpha\beta})$ by (Cammarata, 1994; Nix and Gao, 1998)

$$\sigma^s_{\alpha\beta} = \frac{\partial \mathscr{G}}{\partial \varepsilon^s_{\alpha\beta}} + \tau_0 \delta_{\alpha\beta}, \tag{1}$$

where $\varepsilon^{s}_{\alpha\beta}$ is the (2×2) surface strain tensor, $\delta_{\alpha\beta}$ is the Kronecker delta for surfaces and the constant τ_0 is the residual surface tension. Eq. (1) can be interpreted as modeling the surface between the a spherical inhomogeneity and the matrix as an elastic skin, or interfacial thin layer that is stretched over the bulk of two sides. In general the interface properties are anisotropic, e.g. dependent on crystallographic directions. Here in the sequel, the interface is taken as elastically isotropic. The effect of residual tension τ_0 is not considered here, but will be revisited in the future. The surface moduli can then be characterized by the surface Lame constants λ_s and μ_s as (Sharma et al., 2003; Sharma and Ganti, 2004)

$$\sigma^{s}_{\beta\alpha} = 2\mu_s\varepsilon^{s}_{\beta\alpha} + \lambda_s\varepsilon^{s}_{\gamma\gamma}\delta_{\beta\alpha}. \tag{2}$$

Conventional summation rules apply unless otherwise stated. The surface moduli λ_s, μ_s have the dimensions of N/m which is different from the standard Lame constants (N/m^2). Note that the Greek indices take on values of interfacial components α, β, $\gamma = \theta$ and φ.

Determination of a constitutive equation of a free surface often requires extensive atomistic simulations. Here we rely on the continuum-based derivation by Miller and Shenoy (2000), and assume that the surface (interface) constitutive relation between the two distinct regions (the inclusion and the matrix) can be characterized by Eq. (2). In this paper we will assume that the surface moduli are known a priori. Nevertheless, we mention that this interface constitutive behavior is in fact contributed by the surface effects from the inclusion side as well as from the matrix part, which is intrinsically homogeneized in a certain way on a nanoscale. Given the surface properties of the inclusion and matrix, we propose in Appendix A a simple approach to simulate the effective surface moduli between the two different regions.

The inclusion and the matrix are both elastically isotropic, characterized by the constitutive relation:

$$\sigma^{k}_{ij} = \left(K_k - \frac{2}{3}\mu_k\right)\delta_{ij}\varepsilon^{k}_{mm} + 2\mu_k\varepsilon^{k}_{ij} - 3\alpha_k K_k\Delta T, \tag{3}$$

where the index $k = i, m$ denotes the inclusion and the the matrix respectively, K is the bulk modulus, μ is the shear modulus, α is the thermal expansion coefficient, δ_{ij} is the Kronecker delta, ΔT is the uniform temperature change and the indices i, j takes on values of 1, 2, 3. Within the framework of small infinitesimal deformation, the strain components ε_{ij} are related to the displacement fields u_i as $\varepsilon_{ij} = (u_{i,j} + u_{j,i})/2$.

2.1. Spherically symmetric deformation

We consider a composite sphere consisting of a spherical core (inhomogeneity) fitting inside a concentric spherical shell (matrix), with a core radius a and exterior radius b. Suppose now that the composite sphere is subjected to a hydrostatic deformation on the outer boundary of the matrix

$$u_r|_{r=b} = e_0 r, \tag{4}$$

together with a uniform temperature change ΔT. Due to symmetry, the deformation is independent of the circumferential and azimuthal directions, θ and φ. That is $u^{k}_{r} = u_k(r)$, $u^{k}_{\theta} = 0$ and $u^{k}_{\varphi} = 0$. We can then derive the free energy of the composite sphere, incorporating the surface effects, as (Sharma et al., 2003)

$$\Pi = \int_0^a\int_0^{2\pi}\int_0^{\pi}\Psi_f r^2\sin\varphi\,\mathrm{d}\varphi\,\mathrm{d}\theta\,\mathrm{d}r + \int_a^b\int_0^{2\pi}\int_0^{\pi}\Psi_m r^2\sin\varphi\,\mathrm{d}\varphi\,\mathrm{d}\theta\,\mathrm{d}r + \int_0^{2\pi}\int_0^{\pi}\Psi_s a^2\sin\varphi\,\mathrm{d}\varphi\,\mathrm{d}\theta, \tag{5}$$

where the bulk and surface elastic energy densities are functions of r, expressed as

$$\Psi_k(r, u_k(r), u'_k(r)) = \frac{1}{2}\sigma^{k}_{ij}(\varepsilon^{k}_{ij} - \alpha_k\delta_{ij}\Delta T), \quad \Psi_s(u_s) = \int_0^{\varepsilon^{s}_{ij}}\sigma^{s}_{ij}\,\mathrm{d}\varepsilon^{s}_{ij}, \tag{6}$$

and the prime denotes derivatives with respect to r. The displacement fields need to fulfill the prescribed boundary condition (4). By setting the variation of the free energy to be zero, i.e., $\delta\Pi = 0$, we obtain the Euler–Lagrange equation

$$r^2\frac{\mathrm{d}^2u_k}{\mathrm{d}r^2} + 2r\frac{\mathrm{d}u_k}{\mathrm{d}r} - 2u_k = 0, \tag{7}$$

together with the interface conditions

$$u_i(r)|_{r=a} = u_m(r)|_{r=a}, \quad \sigma^m_{rr} - \sigma^i_{rr} = \left.\frac{2\sigma^s_{\theta\theta}}{r}\right|_{r=a}. \tag{8}$$

This framework is valid for a composite sphere with isotropic constituents and the surface relation (2) together with the thermal effects. Note that in the absence of thermal effects the interface conditions remain the same. The governing field (7), together with the interface conditions (8) and the boundary condition (4), will allow us to determine the field solutions.

2.2. Transverse shear deformation

Next we consider a transverse shear deformation, in which the boundary condition, $u_x = cx$, $u_y = -cy$, $u_z = 0$, is prescribed on the matrix boundary $r = b$. Here b could be infinity. In terms of spherical coordinates, it is equivalent to $u_r = cr\sin^2\varphi\cos 2\theta$, $u_\varphi = cr\sin\varphi\cos\varphi\cos 2\theta$, $u_\theta = -cr\sin\varphi\sin 2\theta$, where c is the maximum value of shear strain. The displacement fields of the composite sphere under the condition can be expressed as (Christensen and Lo, 1979):

$$u^k_r = U_k(r)\sin^2\varphi\cos 2\theta, \quad u^k_\varphi = V_k(r)\sin\varphi\cos\varphi\cos 2\theta, \quad u^k_\theta = W_k(r)\sin\varphi\sin 2\theta, \tag{9}$$

where $U_k(r)$, $V_k(r)$ and $W_k(r)$ are unknown functions of r. The non-vanishing strain components are:

$$\begin{aligned}
&\varepsilon^k_r = \frac{dU_k}{dr}\sin^2\varphi\cos 2\theta, \quad \varepsilon^k_\varphi = \frac{1}{r}\cos 2\theta(U_k\sin^2\varphi + V_k\cos 2\varphi),\\
&\varepsilon^k_\theta = \frac{\cos 2\theta}{r}(2W_k + U_k\sin^2\varphi + V_k\cos^2\varphi), \quad 2\varepsilon^k_{r\varphi} = \frac{\sin 2\varphi}{2}\cos 2\theta\left(\frac{2}{r}U_k - \frac{1}{r}V_k + \frac{dV_k}{dr}\right),\\
&\varepsilon^s_{\varphi\varphi} = \varepsilon^k_{\varphi\varphi}(a,\varphi,\theta), \quad \varepsilon^s_{\theta\theta} = \varepsilon^k_\theta(a,\varphi,\theta), \quad \varepsilon^s_{\theta\varphi} = \varepsilon^k_{\theta\varphi}(a,\varphi,\theta),\\
&2\varepsilon^k_{\theta\varphi} = -\frac{2}{r}V_k\cos\varphi\sin 2\theta, \quad 2\varepsilon^k_{r\theta} = \sin\varphi\sin 2\theta\left(\frac{dW_k}{dr} - \frac{W_k}{r} - \frac{2U_k}{r}\right),
\end{aligned} \tag{10}$$

and the corresponding stresses can be derived from (3). Again the interface between the inclusion and the matrix is endowed with a deformation dependent interfacial energy. The free energy of the composite system Π was given in (5), without considering the temperature term in (6). Note that, in contrast to the axisymmetric loadings, the strain energy density now depends on the radial direction r as well as on θ and φ. Setting $\delta\Pi = 0$ and allowing that the variations $\delta U_k(r)$, $\delta V_k(r)$ and $\delta W_k(r)$ be arbitrarily varied, one finds the Euler–Lagrange equations (three dependent variables with one independent variable, see Hildebrand (1965)

$$\frac{\partial F_k}{\partial U_k} - \frac{\partial}{\partial r}\left(\frac{\partial F_k}{\partial U'_k}\right) = 0, \quad \frac{\partial F_k}{\partial V_k} - \frac{\partial}{\partial r}\left(\frac{\partial F_k}{\partial V'_k}\right) = 0, \quad \frac{\partial F_k}{\partial W_k} - \frac{\partial}{\partial r}\left(\frac{\partial F_k}{\partial W'_k}\right) = 0, \tag{11}$$

where

$$F_k(r, U_k, U'_k, V_k, V'_k) = \int_0^{2\pi}\int_0^{\pi} r^2\Psi_k\sin\varphi\, d\varphi\, d\theta, \quad \text{with } \Psi_k(r,\theta,\varphi) = \frac{1}{2}\sigma^k_{ij}\varepsilon^k_{ij}. \tag{12}$$

We mention that the strain components and the corresponding stresses can be found from (10) and (3). After some tedious algebra, the integral F_k can be integrated as

$$\begin{aligned}
F_k = \frac{2\pi}{15}\{&4U_k[2(2\lambda_k + 5\mu_k)U_k - (2\lambda_k + 3\mu_k)(V_k - 5W_k) + r(4\lambda_k U'_k + \mu_k V'_k - 5\mu_k W'_k)]\\
&+ 4r^2(\lambda_k + 2\mu_k)U'^2_k + V_k[3(2\lambda_k + 7\mu_k)V_k + 20\mu_k W_k - 2r(2\lambda_k U'_k + \mu_k V'_k)]\\
&+ r^2\mu_k V'^2_k + 5W_k[(6\lambda_k + 13\mu_k)W_k + 2r(\lambda_k V'_k - \mu_k W'_k)] + 5r^2\mu_k W'^2\},
\end{aligned} \tag{13}$$

where λ and μ are Lamé's constants. Upon substitution of (13) into (11), we find the system of governing equations

$$\begin{cases} 2\dfrac{1-v_k}{1-2v_k}\left(U_k''+\dfrac{2}{r}U_k'-\dfrac{2}{r^2}U_k-\dfrac{3}{r}V_k'+\dfrac{3}{r^2}V_k\right)+\left(-\dfrac{6}{r^2}U_k+\dfrac{3}{r}V_k'+\dfrac{3}{r^2}V_k\right)=0, \\ 2\dfrac{1-v_k}{1-2v_k}\left(\dfrac{2}{r}U_k'+\dfrac{4}{r^2}U_k-\dfrac{6}{r^2}V_k\right)+\left(-\dfrac{2}{r}U_k'+V_k''+\dfrac{2}{r}V_k'\right)=0, \\ V_k+W_k=0, \end{cases} \tag{14}$$

where v_k denotes the Poisson's ratio for phase k. We note that the system, (14), is the same as that of the composite system with perfectly bonded interface (Christensen and Lo, 1979). Of course, the system of equations (14) can also be derived by substituting (9) into the equilibrium equations.

To proceed, we note that the functions U_m, V_m and W_m need to comply with the boundary conditions, which imply that $\delta U_m=\delta V_m=\delta W_m=0$ at $r\to b$. In addition, to avoid rigid body translation we set $U_i=V_i=W_i=0$ at $r=0$. Also we require that the minimizing functions U, V and W need to be continuous at the interface $r=a$

$$U_i(a)=U_m(a),\quad V_i(a)=V_m(a),\quad W_i(a)=W_m(a). \tag{15}$$

The remaining boundary terms of $\delta\Pi$ becomes

$$\left(\frac{\partial F_i}{\partial U_i'}\delta U_i+\frac{\partial F_i}{\partial V_i'}\delta V_i+\frac{\partial F_i}{\partial W_i'}\delta W_i\right)\Bigg|_{r\to a}-\left(\frac{\partial F_m}{\partial U_m'}\delta U_m+\frac{\partial F_m}{\partial V_m'}\delta V_m+\frac{\partial F_m}{\partial W_m'}\delta W_m\right)\Bigg|_{r\to a}+\delta F_{\mathrm{s}}=0, \tag{16}$$

where

$$\begin{aligned} F_{\mathrm{s}} &= a^2\int_0^{2\pi}\int_0^{\pi}\int_0^{\varepsilon_{ij}^{\mathrm{s}}}\sigma_{ij}^{\mathrm{s}}\,\mathrm{d}\varepsilon_{ij}^{\mathrm{s}}\sin\varphi\,\mathrm{d}\varphi\,\mathrm{d}\theta \\ &= a^2\int_0^{2\pi}\int_0^{\pi}\left\{\frac{1}{2}(\lambda_{\mathrm{s}}+2\mu_{\mathrm{s}})((\varepsilon_{\varphi\varphi}^{\mathrm{s}})^2+(\varepsilon_{\theta\theta}^{\mathrm{s}})^2)+\lambda_{\mathrm{s}}\varepsilon_{\varphi\varphi}^{\mathrm{s}}\varepsilon_{\theta\theta}^{\mathrm{s}}+2\mu_{\mathrm{s}}(\varepsilon_{\varphi\theta}^{\mathrm{s}})^2\right\}\sin\varphi\,\mathrm{d}\varphi\,\mathrm{d}\theta. \end{aligned} \tag{17}$$

Eq. (16) is exactly the natural transition conditions in theory of variation (Hildebrand, 1965, p. 129). Upon substitution of (13) into (16), we find the interfacial jump conditions

$$\hat{\sigma}_{rr}^{m}(r)-\hat{\sigma}_{rr}^{i}(r)|_{r\to a}=\frac{2(\lambda_{\mathrm{s}}+\mu_{\mathrm{s}})(2U_{\mathrm{s}}-3V_{\mathrm{s}})}{r}\Bigg|_{r\to a}, \tag{18}$$

$$\hat{\sigma}_{r\varphi}^{m}(r)-\hat{\sigma}_{r\varphi}^{i}(r)|_{r\to a}=-2\frac{[\lambda_{\mathrm{s}}(2U_{\mathrm{s}}-3V_{\mathrm{s}})+\mu_{\mathrm{s}}(2U_{\mathrm{s}}-5V_{\mathrm{s}})]}{r}\Bigg|_{r\to a}, \tag{19}$$

$$\hat{\sigma}_{r\theta}^{m}(r)-\hat{\sigma}_{r\theta}^{i}(r)|_{r\to a}=2\frac{[\lambda_{\mathrm{s}}(2U_{\mathrm{s}}-3V_{\mathrm{s}})+\mu_{\mathrm{s}}(2U_{\mathrm{s}}-5V_{\mathrm{s}})]}{r}\Bigg|_{r\to a}, \tag{20}$$

where the hat quantities, independent of φ and θ, are given by

$$\begin{aligned} &\sigma_{rr}^{k}(r,\theta)=\hat{\sigma}_{rr}^{k}(r)\frac{\sin^2\varphi\cos 2\theta}{a},\quad \sigma_{r\varphi}^{k}(r,\theta)=\hat{\sigma}_{r\varphi}^{k}(r)\frac{\sin\varphi\cos\varphi\cos 2\theta}{a}, \\ &\sigma_{r\theta}^{k}(r,\theta)=\hat{\sigma}_{r\theta}^{k}(r)\frac{\sin\varphi\sin 2\theta}{a}. \end{aligned} \tag{21}$$

Note that $V=-W$ and $\hat{\sigma}_{r\theta}^{k}=-\hat{\sigma}_{r\varphi}^{k}$. Thus in resolving the boundary value problem, only U and V can be treated as unknowns and the interface conditions involved are $(15)_{1,2}$, (18) and (19). Conditions (18), (19) can be further simplified as

$$\sigma_{rr}^{m}(r)-\sigma_{rr}^{i}(r)|_{r\to a}=\frac{\sigma_{\varphi\varphi}^{\mathrm{s}}+\sigma_{\theta\theta}^{\mathrm{s}}}{r}\Bigg|_{r\to a}, \tag{22}$$

$$\sigma_{r\varphi}^{m}(r)-\sigma_{r\varphi}^{i}(r)|_{r\to a}=\frac{1}{r}\frac{\partial(\sigma_{\theta\theta}^{\mathrm{s}}-\sigma_{\varphi\varphi}^{\mathrm{s}})}{\partial\varphi}-\frac{\sigma_{\varphi\varphi}^{\mathrm{s}}+\sigma_{\theta\theta}^{\mathrm{s}}}{r}\cot\varphi\Bigg|_{r\to a}. \tag{23}$$

Similar expressions can also be found in a recent paper (Wang et al., 2005), which are deduced from the generalized Young–Laplace equation for an orthogonal curvilinear system (Duan et al., 2005b). When setting $\lambda_s = \mu_s = 0$, the mathematical framework will recover the known equations for perfect bonding.

3. Exact size-dependent connection between bulk modulus and thermal expansion coefficient

For two-phase composites with particle reinforcements, it is well known that there exist exact connections between the overall bulk modulus and the effective thermal expansion coefficient (Levin, 1967; Benveniste and Dvorak, 1990). Here, we will show that for a composite medium consisting of many spherical inclusions of the same size with surface effects (λ_s, μ_s) prevailing along the interfaces, an analogous type of exact connection also exists. The spherical inclusions can be arbitrarily distributed in the matrix, or arranged in a periodic manner. In the former situation the overall behavior of the composite will be effectively isotropic.

Let us now consider that a representative volume V of the composite medium, which will be used to characterize the overall behavior of the composite. We first prove that under a certain loading path that includes a uniform temperature change θ_0, a hydrostatic deformation field

$$u_x = e_0 x, \quad u_y = e_0 y, \quad u_z = e_0 z, \tag{24}$$

is admissible in the entire composite medium. Note that (24) implies that each sphere in the composite is now subjected to a uniform hydrostatic deformation

$$\varepsilon_{rr} = \varepsilon_{\theta\theta} = \varepsilon_{\varphi\varphi} = e_0. \tag{25}$$

When (24) prevails, then the interface condition $(8)_1$ is automatically fulfilled. The remaining condition to be satisfied is $(8)_2$. To proceed, we note from (25) and (2) that $\sigma^s_\theta = 2(\lambda_s + \mu_s)e_0$. Thus condition $(8)_2$ can be written as

$$\left(K_i - K_m + \frac{4(\lambda_s + \mu_s)}{3a}\right)e_0 = (K_i\alpha_i - K_m\alpha_m)\Delta T. \tag{26}$$

This algebraic condition (26) implies that when the external deformation e_0 and the temperature change ΔT are properly adjusted, then a homogeneous deformation (25) does exist in the whole composite medium.

Next, we derive the average stress and strain of the composite. The overall thermoelastic behavior of the composite with interface stress is elastically isotropic. The overall properties consists of the effective bulk modulus K^*, the effective shear modulus μ^* and the effective thermal expansion coefficient α^*. The average stresses and average strains are related by the relation

$$\begin{gathered}\begin{pmatrix}\bar\sigma_r\\ \bar\sigma_\varphi\\ \bar\sigma_\theta\end{pmatrix} = \begin{pmatrix} K^* + \frac{4}{3}\mu^* & K^* - \frac{2}{3}\mu^* & K^* - \frac{2}{3}\mu^* \\ & K^* + \frac{4}{3}\mu^* & K^* - \frac{2}{3}\mu^* \\ SYM & & K^* + \frac{4}{3}\mu^* \end{pmatrix}\begin{pmatrix}\bar\varepsilon_r - \alpha^*\Delta T\\ \bar\varepsilon_\varphi - \alpha^*\Delta T\\ \bar\varepsilon_\theta - \alpha^*\Delta T\end{pmatrix},\\ \bar\sigma_{r\varphi} = 2\mu^*\bar\varepsilon_{r\varphi}, \quad \bar\sigma_{\theta\varphi} = 2\mu^*\bar\varepsilon_{\theta\varphi}, \quad \bar\sigma_{r\theta} = 2\mu^*\bar\varepsilon_{r\theta},\end{gathered} \tag{27}$$

where the overbar denotes the volume average of the composite. The volume averages of composites with various types of inperfect interfaces were derived by Benveniste and Miloh (2001). In our case, the average fields can be recorded as

$$\begin{aligned}&\bar\varepsilon_{ij} = c_i\bar\varepsilon^i_{ij} + c_m\bar\varepsilon^m_{ij},\\ &\bar\sigma_{ij} = c_i\bar\sigma^i_{ij} + c_m\bar\sigma^m_{ij} - \frac{c_i}{V_i}\int_\Gamma(\sigma^i_{ir} - \sigma^m_{ir})n_r x_j \,\mathrm{d}\Gamma,\end{aligned} \tag{28}$$

where V_i is the volume of the inclusion, $\mathbf{n}$ is the outward normal of the interface, Γ denotes the interface and c_i is the volume fraction of the inclusion. Since the strains and the stresses are spatially uniform inside the inclusion, the fields are exactly equal to their average quantities. Further, noting that the field is purely hydrostatic, the surface integral can be evaluated as

$$\frac{c_i}{V_i}\int_{\Gamma}(\sigma^i_{ir}-\sigma^m_{ir})n_r x_j\,\mathrm{d}\Gamma=-c_i\frac{4(\lambda_s+\mu_s)}{a}e_0. \tag{29}$$

Now use of the uniform field (25) into (28) will provide

$$\sum_{k=i,m}c_kK_k(e_0-\alpha_k\Delta T)+c_i\frac{4(\lambda_s+\mu_s)}{3a}e_0=K^*(e_0-\alpha^*\Delta T). \tag{30}$$

Upon the substitution of condition (26), we can find the exact condition that links the effective bulk modulus K^* and the effective thermal expansion coefficient α^*:

$$\frac{\alpha^*K^*-\left(\sum\limits_{k=i,m}c_k\alpha_kK_k\right)}{K^*-\left(\sum\limits_{k=i,m}c_kK_k\right)-c_i\frac{4(\lambda_s+\mu_s)}{3a}}=\frac{\alpha_iK_i-\alpha_mK_m}{K_i-K_m+\frac{4(\lambda_s+\mu_s)}{3a}}. \tag{31}$$

This equality can be viewed as a generalization of Levin's formula (1967) to the considered composite system with surface effects. It is noted that with the knowledge of effective properties K^*, one can uniquely determine the coefficient α^*.

4. Effective elastic properties

In this section we will derive the effective bulk modulus K^* using the concept of neutral inhomogeneities (Milton, 2002, Chapter 7). The idea of neutral inhomogeneity is mathematically equivalent to that of composite sphere assemblages (CSA) (Hashin, 1962). We mention that for perfect bonding of interfaces (i.e., without surface effect), the effective bulk modulus of the CSA has the same form as that predicted by the Mori–Tanaka method and lies within variational bounds (Benveniste, 1987). For the effective transverse shear μ^*, the CSA does not satisfy consistency conditions, hence the generalized self-consistent method of Christensen and Lo (1979) will be employed to derive the effective transverse shear modulus.

4.1. Effective bulk modulus K^*

We first consider the composite sphere is under the loading (4). The admissible displacement fields, by solving (7), can be written as

$$u^i_r=Ar,\quad u^m_r=Br+\frac{C}{r^2},\quad u^i_\varphi=u^m_\varphi=0,\quad u^i_\theta=u^m_\theta=0, \tag{32}$$

where the coefficients A, B, C are constants that can be determined from the boundary and interface conditions, (4) and (8). Next we consider a homogeneous sphere of the same size as the composite sphere, with the bulk moduli being denoted by K^*. Under the same boundary condition (4), we wish to adjust the values of K^* so that the radial stress at $r=b$ is the same with that of the composite sphere. The effective bulk modulus K^* can then be exactly derived as

$$K^*=K_m+c_i\frac{K_i-K_m+\dfrac{4(\lambda_s+\mu_s)}{3a}}{1+c_m\left(\dfrac{K_i-K_m}{K_m+\frac{4}{3}\mu_m}+\dfrac{4(\lambda_s+\mu_s)}{3a\left(K_m+\frac{4}{3}\mu_m\right)}\right)}. \tag{33}$$

When setting $\lambda_s=\mu_s=0$, it is seen that the formulae for K^* recovers the known classical expression for the perfect bonding situation (Hill, 1963). Using a different procedure, Duan et al. (2005a, Eq. (39)) derived another equivalent form of (33).

4.2. Effective shear modulus μ^*

For the transverse shear loading, it is not possible to find a neutral composite sphere. A commonly adopted procedure in micromechanics literature to assess the transverse shear modulus is through the generalized self-consistent method. This model assumes that the inclusion is first surrounded by some matrix material, and then embedded in an effective medium with unknown effective shear modulus. The auxiliary boundary value problem to be solved is that of a composite sphere with a spherical core with a matrix shell embedded in the unknown effective medium (designated by $*$), and subjected at the remote boundary to a transverse shear boundary condition $u_x|_{r\to\infty} = cx$, $u_y|_{r\to\infty} = -cy$, $u_z = 0$. Under the deformation, the corresponding solutions to (14) have the forms

$$U_r^i = A_1 r - \frac{6v_i}{1-2v_i}A_2 r^3, \quad U_\theta^i = A_1 r - \frac{7-4v_i}{1-2v_i}A_2 r^3, \tag{34}$$

$$U_r^m = B_1 r - \frac{6v_m}{1-2v_m}B_2 r^3 + 3B_3 r^{-4} + \frac{5-4v_m}{1-2v_m}B_4 r^{-2}, \tag{35}$$

$$U_\theta^m = B_1 r - \frac{7-4v_m}{1-2v_m}B_2 r^3 - 2B_3 r^{-4} + 2B_4 r^{-2},$$

$$U_r^* = D_1 r + 3D_3 r^{-4} + \frac{5-4v^*}{1-2v^*}D_4 r^{-2}, \quad U_\theta^* = D_1 r - 2D_3 r^{-4} + 2D_4 r^{-2}, \tag{36}$$

and $U_\varphi^k = -U_\theta^k$. The coefficient D_1 is specified directly by the condition of uniform shear strain at infinite distance from the origin. Next we consider a homogeneous comparison medium, with effective shear modulus μ^*, subjected to the same boundary condition. This will give the referenced field

$$\begin{aligned} &u_r^* = D_1 r\cos 2\theta \sin^2\varphi, \quad u_\theta^* = D_1 r\cos 2\theta \sin\varphi\cos\varphi, \quad u_\varphi^* = D_1 r\sin 2\theta\sin\varphi, \\ &\sigma_r^* = 2\mu^* D_1\cos 2\theta\sin^2\varphi, \quad \sigma_{r\theta}^* = 2\mu^* D_1\cos 2\theta\sin\varphi\cos\varphi, \quad \sigma_{r\varphi}^* = -2\mu^* D_1\sin 2\theta\sin\varphi. \end{aligned} \tag{37}$$

To proceed, we employ the Eshelby's formula (1961) for the strain energy of the system

$$\int_0^{2\pi}\int_0^{\pi}(\sigma_r^* u_r + \sigma_{r\theta}^* u_\theta + \sigma_{r\varphi}^* u_\varphi - \sigma_r u_r^* - \sigma_{r\theta}u_\theta^* - \sigma_{r\varphi}u_\varphi^*)b^2\sin\varphi\,d\varphi\,d\theta = 0. \tag{38}$$

Upon a substitution of the field quantities into the identity (38), it can be proven analytically through the software Mathematica that $D_4 = 0$. This condition is the same with the classical perfect bonding situation. To find μ^*, Christensen and Lo (1986) suggested that one may set $D_4 = 0$ in (36) at the outset, this will remove the dependence of v^* and only the unknown shear modulus μ^* will enter the field solutions. So in total there are eight constants, A_1, A_2, B_1, B_2, B_3, B_4, D_3, μ^*, that will be determined from the eight interface conditions:

$$\begin{aligned} &u_r^i|_{r=a} = u_r^m|_{r=a}, \quad u_r^m|_{r=b} = u_r^*|_{r=b}, \quad u_\theta^i|_{r=a} = u_\theta^m|_{r=a}, \\ &u_\theta^m|_{r=b} = u_\theta^*|_{r=b}, \quad \sigma_r^m|_{r=b} = \sigma_r^*|_{r=b}, \quad \sigma_{r\theta}^m|_{r=b} = \sigma_{r\theta}^*|_{r=b}, \end{aligned} \tag{39}$$

and the interface jump conditions (18) and (19). In the continuity conditions, we have invoked the conditions that u_θ^k and u_φ^k and, also $\sigma_{r\theta}^k$ and $\sigma_{r\varphi}^k$, are dependent. For completeness, we have listed the system of equations in Appendix B. Note that the system is not exactly a linear algebraic set. But the system can be first expressed as a (7×7) linear set plus one additional constraint. The equations listed in (A.4) and (A.5) are exactly the eight interface conditions of (39). The unknown shear modulus μ^* can be found in the form of a linear quadratic algebraic equation. In the absence of the surface effects, we have checked analytically that our equations exactly agree with that of Christensen and Lo (1979). In the presence of surface effects, there is agreement with the self-consistent estimates obtained by Duan et al. (2005a). Note that the thermal expansion coefficients have no effect on the overall elastic moduli, but may contribute an overall transformation (thermal) strain or eigenstrain.

5. Discussions and numerical results

Simple, explicit formulae have been derived for the effective bulk modulus and the thermal expansion coefficient. Interestingly, we find that if we regard

$$K_i + \frac{4(\lambda_s + \mu_s)}{3a} \rightarrow \widetilde{K}_i \tag{40}$$

as the bulk modulus of a replacement inclusion $\widetilde{K}_i$, then formulae (31) and (33) follow exactly the same form as those of the classical results (without interface effects). Therefore, to see if the surface effect is significant, one may simply evaluate the quantity $4(\lambda_s + \mu_s)/(3a)$ and compare the value with that of K_i. It should be mentioned that substitution (40) holds only for the overall moduli K^* and α^* and does not apply to phase bulk moduli. In numerical demonstrations, the free surface properties, generally vary with different crystallographic orientations, are taken from the papers (Sharma and Ganti, 2004; Miller and Shenoy, 2000). Two different sets of surface properties corresponding to the crystallographic directions [1 0 0] and [1 1 1] of Al are recorded. The parameters are: surface A, $\lambda_s = 3.48912$ N/m, $\mu_s = -6.2178$ N/m for [1 0 0] crystallographic direction and surface B, $\lambda_s = 6.842$ N/m, $\mu_s = -0.3755$ N/m for [1 1 1] direction. Surface A has the surface elastic modulus $K_s = 2(\lambda_s + \mu_s)$, equal to -5.457 N/m, while surface B has $K_s = 12.932$ N/m. We mention that in most cases the surface energy is positive, but the surface moduli can be negative (see for instance, Gurtin et al., 1998, p. 1105). Discussions on negative surface energy in a multicomponent system can be found in Lodziana et al. (2004) and Marthus et al. (2005). For comparison with classical results, we shall use the index C to denote the surface for classical perfect bonding solutions (without interface stress). We mention that the surface moduli can be non-positive. Since the typical value of the bulk modulus is of the order of GPa, thus the surface term can take effect only if the radius of the inclusion is in the order of nanometer (nm). When compared with the perfectly bonded interface, surface A conditions are seen to render a negative value of and thus reduce the overall bulk modulus. Surface conditions B have an opposite effect.

The numerical calculations illustrate the role of surface effects in an aluminum matrix containing nano-size cavities with surface effects on the cavity boundary at $r = a$, with $K_i = \mu_i = 0$. In particular, we evaluate the transverse shear modulus and the linear coefficient of thermal expansion of a cavitated matrix. The matrix properties are those suggested by Duan et al. (2005a), with $K_m = 75.2$ GPa, $v_m = 0.3$, $\alpha_m = 9.3 \times 10^{-6}$ 1/°C. Under hydrostatic loading, the field solutions for this problem can be derived from (7) and (8). Detailed results appear in the papers by Sharma and Ganti (2004) and Sharma et al. (2003) and will not be repeated here. Under transverse shear deformation prescribed here as $u_x|_{x\to\infty} = D_1 x$, $u_y|_{r\to\infty} = -D_1 y$, $u_z = 0$, we develop the details of the solution in Appendix C. The maximum hoop stress $\sigma_{\theta\theta}$ occurs at the points $\varphi = \pi/2, \theta = 0$ or π on the boundary of the cavity. Fig. 1 shows the ratio of $\max\sigma_{\theta\theta}$ at $r = a$ versus the corresponding quantity

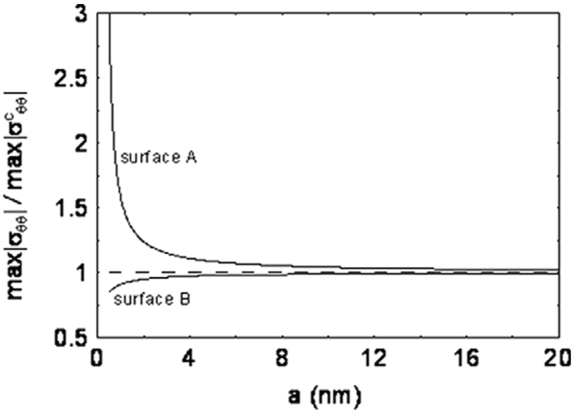

Fig. 1. $\max\sigma_{\theta\theta}$ for a spherical cavity in an unbounded matrix containing under a remote transverse shear deformation. The surface A is calculated based on the surface property of Al [1 0 0], surface B uses the surface moduli of Al [1 1 1] and the index C denotes the classical elasticity solution without surface effect.

without the surface effects (denoted as max $\sigma_{\theta\theta}^{C}$). For surface A, the stress concentration increases as the cavity becomes small. Surface B reverses the trend. Fig. 2 presents the ratio μ^*/μ_C^* as a function of cavity radius a (in nm) for cavity volume fraction $c_i = 0.3$. The effective bulk moduli shown in Sharma and Ganti (2004) show a similar trend. The surface effect becomes negligible when the radius of the cavity is larger than 50 nm. Fig. 3 shows the effect of cavity radius on the ratio α^*/α_C^* of the modified to classical expansion coefficients. In Fig. 4, we vary the volume fraction of the spherical cavities to assess its influence on the effective μ^* for two different surface properties. Two different radii of the cavity are selected, $a = 5$ nm and $a = 20$ nm. When the size of the inclusions is small, the surface effects become pronounced. Fig. 5 plots the value of α^*/α_C^* versus the volume fraction of spherical cavities with two different radii of the cavity and two different surface properties.

In summary, we have illustrated the effect of surface stresses on local filed and overall moduli of a solid containing nano-sized cavities. Variational procedures were used to construct the governing system together with the interface conditions. Hydrostatic and deviatoric deformations are considered separately. Simple expressions for evaluations of the effective bulk modulus and thermal expansion coefficient are derived. We have presented a proof of an exact size-dependent connection between the effective thermal expansion coefficient and the effective bulk modulus. This result is valid for a general composite containing many spheres of the same radius, not just restricted to a composite sphere. The proof is based upon the existence of a uniform isotropic deformation field in the whole composite medium, created by specific mechanical and transformation loads. The transverse shear modulus is derived using the generalized self-consistent method.

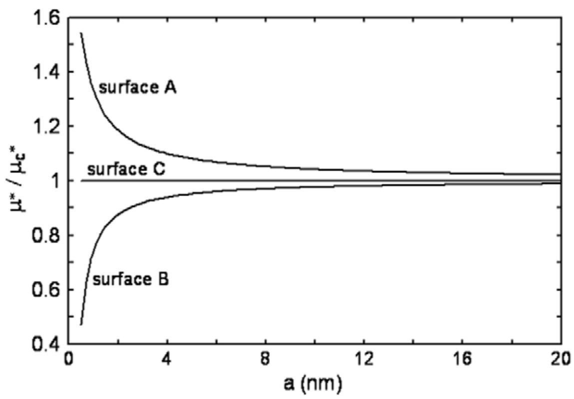

Fig. 2. The value of μ^*/μ_C^* versus the radius of the spherical cavity a (nm) for the volume fraction $c_i = 0.3$ using the generalized self-consistent method. The value μ_C^* denotes the effective shear modulus of a medium containing spherical cavities without surface effect.

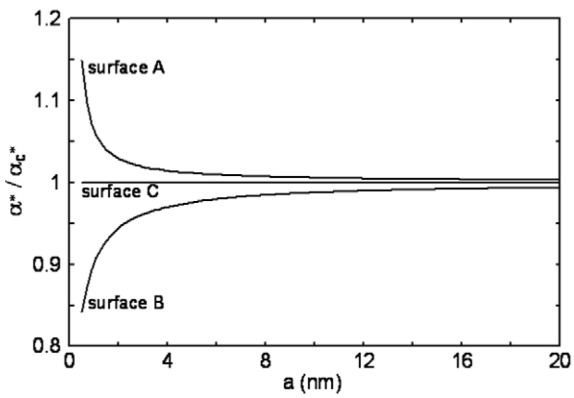

Fig. 3. The value of α^*/α_C^* versus the radius of the spherical cavity a (nm) for the volume fraction $c_i = 0.3$. The value α_C^* denotes the effective thermal expansion coefficient of a medium containing spherical cavities without surface effect.

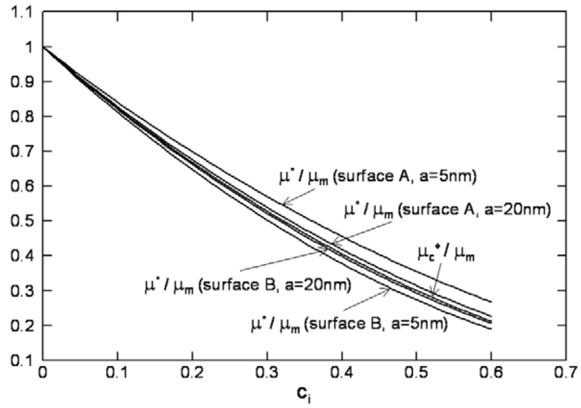

Fig. 4. The values of μ^*/μ_m and μ_C^*/μ_m versus the volume fraction c_i for a medium containing spherical cavities of sizes $a = 5$ nm and $a = 20$ nm with surface properties A or B. The μ_C^*/μ_m line was computed for a porous medium without surface effects.

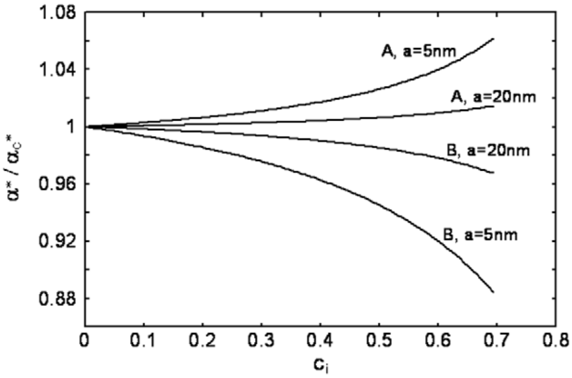

Fig. 5. The value of α^*/α_C^* versus the volume fraction c_i of the spherical cavity for $a = 5$ nm and $a = 20$ nm. The value α_C^* denotes the effective thermal expansion coefficient of a medium containing spherical cavities without surface effect.

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Appendix A

Let us consider two distinct regions, designated as materials 1 and 2, separated by a spherical boundary. Suppose that the spherical boundary of each region is a free surface, the surface stress and strain relations can be characterized as

$$(\sigma^{\mathrm{s}}_{\beta\alpha})^{(1)} = 2\mu_{\mathrm{s}}^{(1)}(\varepsilon^{\mathrm{s}}_{\beta\alpha})^{(1)} + \lambda_{\mathrm{s}}^{(1)}(\varepsilon^{\mathrm{s}}_{\gamma\gamma})^{(1)}\delta_{\beta\alpha}, \tag{A.1}$$

$$(\sigma^{\mathrm{s}}_{\beta\alpha})^{(2)} = 2\mu_{\mathrm{s}}^{(2)}(\varepsilon^{\mathrm{s}}_{\beta\alpha})^{(2)} + \lambda_{\mathrm{s}}^{(2)}(\varepsilon^{\mathrm{s}}_{\gamma\gamma})^{(2)}\delta_{\beta\alpha}, \tag{A.2}$$

where the subscripts α, $\beta = \theta$ and φ are defined in Section 2. Here μ_{s} and λ_{s} are surface moduli as stated in Section 2 and are assumed to be known, calculated from atomistic simulations or by other approaches. Since the two materials are different, in general we have $\mu_{\mathrm{s}}^{(1)} \neq \mu_{\mathrm{s}}^{(2)}$, $\lambda_{\mathrm{s}}^{(1)} \neq \lambda_{\mathrm{s}}^{(2)}$.

Now suppose that the two materials are bonded together by a coherent interface, which enforces displacement continuity. This assures the surface strains will be identical on both sides of the interface Γ

$$(\varepsilon^{s}_{\beta\alpha})^{(1)}|_{\Gamma} = (\varepsilon^{s}_{\beta\alpha})^{(2)}|_{\Gamma} \equiv \varepsilon^{s}_{\beta\alpha}. \tag{A.3}$$

We mention that the surface strains were also referred to as interior part of strain in the context of interfacial discontinuity (Hill, 1983; Laws, 1975).

Bringing the two surfaces in contact is bound to change their properties. In the present work, we view the two surfaces 1 and 2, as well as their interface, as infinitely thin membranes. We assume that the ”overall” stress in the joined interface is simply the volume average of $\sigma^{s}_{\alpha\beta}$ in materials 1 and 2

$$\sigma^{s}_{\beta\alpha} = w_1(\sigma^{s}_{\beta\alpha})^{(1)} + w_2(\sigma^{s}_{\beta\alpha})^{(2)}, \quad \text{with } w_1 + w_2 = 1, \tag{A.4}$$

and that this stress supersedes those of the two free surfaces in (A.1) and (A.2), and thus applies to both joined surfaces. This result and the magnitudes of $\mathbf{w}_1$ and $\mathbf{w}_2$ should be further justified by atomistic simulations. As pointed out by a referee, such simulations have been performed by Girifalco and Good (1957) and Kitazaki and Hata (1972).

Appendix B

Here we outline the system of algebraic equations for the solution of effective shear modulus μ^* through the generalized self-consistent method. Without loss of generality we can set $D_1 = 1$. The system of equations can be first written as a linear algebraic set:

$$[\mathbf{A}]_{7\times7}[\mathbf{x}]_{7\times1} = [\mathbf{b}]_{7\times1}, \tag{B.1}$$

where

$$\mathbf{x}^{\mathrm{T}} = [A_1, \widetilde{A}_2, B_1, \widetilde{B}_2, \widetilde{B}_3, \widetilde{B}_4, \widetilde{D}_3], \tag{B.2}$$

$$\mathbf{b}^{\mathrm{T}} = [0, 0, 1, 1, 5\mu^*, 0, 0], \tag{B.3}$$

with $\widetilde{A}_2 = A_2a^2$, $\widetilde{B}_2 = B_2b^2$, $\widetilde{B}_3 = B_3/a^5$, $\widetilde{B}_4 = B_4/a_3$, $\widetilde{D}_3 = D_3/b^5$. The non-vanishing components of $\mathbf{A}$ are

$$\begin{aligned}
&A_{11} = 1, \quad A_{12} = -\frac{6v_i}{1-2v_i}, \quad A_{13} = -1, \quad A_{14} = \frac{6v_m}{1-2v_m}c_i^{2/3}, \quad A_{15} = -3, \quad A_{16} = -\frac{5-4v_m}{1-2v_m},\\
&A_{21} = 1, \quad A_{22} = -\frac{7-4v_i}{1-2v_i}, \quad A_{23} = -1, \quad A_{24} = \frac{7-4v_m}{1-2v_m}c_i^{2/3}, \quad A_{25} = 2, \quad A_{26} = -2,\\
&A_{33} = 1, \quad A_{34} = -\frac{6v_m}{1-2v_m}, \quad A_{35} = 3c_i^{5/3}, \quad A_{36} = \frac{5-4v_m}{1-2v_m}c_i, \quad A_{37} = -3,\\
&A_{43} = 1, \quad A_{44} = -\frac{7-4v_m}{1-2v_m}, \quad A_{45} = -2c_i^{5/3}, \quad A_{46} = 2c_i, \quad A_{47} = 2,\\
&A_{53} = 5\mu_m, \quad A_{54} = 21\left(\lambda_m - \mu_m\frac{1+2v_m}{1-2v_m}\right), \quad A_{56} = -\left(6\lambda_m + \frac{2\mu_m(7-11v_m)}{1-2v_m}\right)c_i,\\
&A_{61} = 2\left(-\mu_i + \frac{\lambda_s+\mu_s}{a}\right), \quad A_{62} = -21\lambda_i + \frac{36v_m\mu_m}{1-2v_m} - 6\frac{\lambda_s+\mu_s}{a}\frac{7-8v_i}{1-2v_i}, \quad A_{63} = 2\mu_m,\\
&A_{64} = \left(21\lambda_m - \frac{36v_m\mu_m}{1-2v_m}\right)c_i^{2/3}, \quad A_{65} = -24\mu_m, \quad A_{66} = -\left(6\lambda_m + \frac{4\mu_m(5-4v_m)}{1-2v_m}\right),\\
&A_{71} = -\mu_i + \frac{\lambda_s+3\mu_s}{a}, \quad A_{72} = \frac{7+2v_i}{1-2v_i}\mu_i - \frac{21-24v_i}{1-2v_i}\frac{\lambda_s}{a} - \frac{35-32v_i}{1-2v_i}\frac{2\mu_s}{a}, \quad A_{73} = \mu_m,\\
&A_{74} = -\frac{7+2v_m}{1-2v_m}\mu_m c^{2/3}, \quad A_{75} = 8\mu_m, \quad A_{76} = 2\mu_m\frac{1+v_m}{1-2v_m}.
\end{aligned} \tag{B.4}$$

The unknown vector $\mathbf{x}$ can be solved in terms of a linear function of μ^* through a symbolic algebriac software (e.g. Mathematica). The solutions of $\widetilde{B}_2, \widetilde{B}_3, \widetilde{B}_4, \widetilde{D}_3$ can then be substituted into the 8th condition for the solution of μ^*:

$$-40c_i^{5/3}\mu_m\widetilde{B}_3 + \left(19K_m + \frac{4}{3}\mu_m\right)\widetilde{B}_2 - 8c_i(3K_m + \mu_m)\widetilde{B}_4 + 40\mu^*\widetilde{D}_3 = 0, \tag{B.5}$$

which will lead to a linear quadratic equation for μ^*.

Appendix C

Here we consider the boundary value problem of a spherical cavity in an unbounded matrix under a remote transverse shear deformation $u_x|_{x\to\infty} = D_1 x$, $u_y|_{r\to\infty} = -D_1 y$, $u_z = 0$. Along the boundary of the cavity ($r = a$) surface effects are considered. From (36), we can write the displacement field in the matrix as

$$\begin{aligned} u_r &= \left(D_1 r + 3\frac{D_3}{r^4} + \frac{5-4v}{1-2v}\frac{D_4}{r^2}\right)\sin^2\varphi\cos 2\theta, \\ u_\varphi &= \left(D_1 r - 2\frac{D_3}{r^4} + 2\frac{D_4}{r^2}\right)\sin\varphi\cos\varphi\cos 2\theta, \\ u_\theta &= -\left(D_1 r - 2\frac{D_3}{r^4} + 2\frac{D_4}{r^2}\right)\sin\varphi\sin 2\theta, \end{aligned} \tag{C.1}$$

where the remote displacement boundary conditions are satisfied and the unknown coefficients D_3 and D_4 are to be determined from the jump condition of traction at $r = a$. The stresses σ_{rr} and $\sigma_{r\varphi}$ corresponding to (C1) can be derived in the forms

$$\begin{aligned} \sigma_{rr} &= \left[-6\lambda\frac{D_4}{r^3} + 2\mu\left(D_1 - 12\frac{D_3}{r^5} - 2\frac{5-4v}{1-2v}\frac{D_4}{r^3}\right)\right]\sin^2\varphi\cos 2\theta, \\ \sigma_{r\varphi} &= \mu\left(D_1 + 8\frac{D_3}{r^5} + 2\frac{1+v}{1-2v}\frac{D_4}{r^3}\right)\sin 2\varphi\cos 2\theta. \end{aligned} \tag{C.2}$$

The two jump conditions (18) and (19) can be expanded as (in the absence of τ_0)

$$\begin{cases} 12\left(\mu + \dfrac{\lambda_s + \mu_s}{a}\right)\dfrac{D_3}{a^5} + \left(9K + 4\mu + \dfrac{6K}{\mu}\dfrac{\lambda_s + \mu_s}{a}\right)\dfrac{D_4}{a^3} = \left(\mu + \dfrac{\lambda_s + \mu_s}{a}\right)D_1, \\ 4\left(2\mu + 3\dfrac{\lambda_s + \mu_s}{a} + \dfrac{\mu_s}{a}\right)\dfrac{D_3}{a^5} + \left(3K + \dfrac{6K}{\mu}\dfrac{\lambda_s + \mu_s}{a} - \dfrac{4\mu_s}{a}\right)\dfrac{D_4}{a^3} = \left(-\mu + \dfrac{\lambda_s + 3\mu_s}{a}\right)D_1. \end{cases} \tag{C.3}$$

The linear algebraic set of equations allows us to determine the coefficients D_3 and D_4 as

$$\frac{D_3}{a^5} = D_1\frac{\mathcal{N}_1}{\Delta}, \quad \frac{D_4}{a^3} = D_1\frac{\mathcal{N}_2}{\Delta}, \tag{C.4}$$

where

$$\Delta = \det\begin{pmatrix} 12\left(\mu + \dfrac{\lambda_s + \mu_s}{a}\right) & 9K + 4\mu + 6\dfrac{K}{\mu}\dfrac{\lambda_s + \mu_s}{a} \\ 4\left(2\mu + 3\dfrac{\lambda_s + \mu_s}{a} + \dfrac{\mu_s}{a}\right) & 3K + 6\dfrac{K}{\mu}\dfrac{\lambda_s + \mu_s}{a} - 4\dfrac{\mu_s}{a} \end{pmatrix}, \tag{C.5}$$

$$\mathcal{N}_1 = \det\begin{pmatrix} \mu + \dfrac{\lambda_s + \mu_s}{a} & 9K + 4\mu + 6\dfrac{K}{\mu}\dfrac{\lambda_s + \mu_s}{a} \\ -\mu + \dfrac{\lambda_s + 3\mu_s}{a} & 3K + 6\dfrac{K}{\mu}\dfrac{\lambda_s + \mu_s}{a} - 4\dfrac{\mu_s}{a} \end{pmatrix}, \tag{C.6}$$

$$\mathscr{N}_2 = \det\begin{pmatrix} 12\left(\mu + \dfrac{\lambda_s + \mu_s}{a}\right) & \mu + \dfrac{\lambda_s + \mu_s}{a} \\ 4\left(2\mu + 3\dfrac{\lambda_s + \mu_s}{a} + \dfrac{\mu_s}{a}\right) & -\mu + \dfrac{\lambda_s + 3\mu_s}{a} \end{pmatrix}. \tag{C.7}$$

In the absence of the surface effects, $\lambda_s = \mu_s = 0$, namely the boundary of the cavity is traction free, the coefficients have the simple forms

$$\frac{D_3}{a^5} = -D_1\frac{3K + \mu}{9K + 8\mu}, \quad \frac{D_4}{a^3} = D_1\frac{5\mu}{9K + 8\mu}. \tag{C.8}$$

The stress concentration on the cavity surface can be evaluated through the hoop stresses

$$\sigma_{\theta\theta} = -2\mu\cos 2\theta\left[\left(D_1 - 2\frac{D_3}{r^5} + 2\frac{D_4}{r^3}\right) - \left(5\frac{D_3}{r^5} + 3\frac{D_4}{r^3}\right)\sin^2\varphi\right], \tag{C.9}$$

$$\sigma_{\varphi\varphi} = 2\mu\cos 2\theta\left[\left(D_1 - 2\frac{D_3}{r^5} + 2\frac{D_4}{r^3}\right) - \left(D_1 - 7\frac{D_3}{r^5} - \frac{D_4}{r^3}\right)\sin^2\varphi\right]. \tag{C.10}$$

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