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# Eshelby formalism for multi-shell nano-inhomogeneities

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NANO-PARTICLES consisting of a core surrounded by multiple outer shells (multi-shell particles) are used as novel functional materials as well as stiffeners/toughners in conventional composites and nanocomposites. In these heterogeneous particles, the mismatch of thermal expansion coefficients and lattice constants between neighboring shells induces stress/strain fields in the core and shells, which in turn affect the physical/mechanical properties of the particles themselves and/or of the composites containing them. In this paper, we solve the elastostatic *inhomogeneous inclusion* problem of an infinite medium containing a multi-shell spherical particle when the eigenstrains are prescribed in the particle and in the multi-shells, and the *inhomogeneity* problem when an arbitrary remote stress field is applied to the infinite medium. The corresponding Eshelby and stress concentration tensors of the two problems are obtained and specialised to inhomogeneous inclusions in finite spherical domains with fixed displacement or traction-free boundary conditions. Finally, the Eshelby tensor of a spherical inhomogeneity with non-uniform eigenstrain is obtained and applied to quantum dots of uniform and non-uniform compositions.

**Key words:** nano-inhomogeneity, multi-shell, non-uniform eigenstrain, Eshelby tensor, finite domain, nano-onions, quantum.

## 1. Introduction

THE SYNTHESIS and characterization of nano-particles with core-shell structures have attracted a lot of attention in many areas of science and technology. These particles which are ellipsoidal or spherical in shape and which consist of a core surrounded by concentric shells of nanometer-size are called "nano-onions" because of this special structure [1, 2]. In order to obtain target properties, different systems, in terms of materials and shell thickness, have been produced (e.g., CdS/HgS/CdS and Cds/HgS/Cds/HgS/Cds) [3, 4]. Multi-fold core-shell structured particles of micrometer-size are called "micro-onions" [5]. In materials science and engineering, the particles with core-shell structures have been used as reinforcements and tougheners in composites [6]. In solid-state physics,

nano-onions are found to exhibit novel physical effects and properties, such as quantum confinement effect, and novel electronic, magnetic and optical properties [7–11]. Nano-onions can be used on their own as functional devices, besides being a constituent part of a composite medium [2, 12–14]. Nano-onions are a kind of quantum dot (QD). The strain distributions in heterogeneous electronic structures of fine scale, e.g., quantum dot (QD) structures, have been extensively studied [15, 16] and it has been shown that the strains affect the optical properties of these structures by modifying the energies and wave functions of the confined carriers. Thus, the knowledge of strain fields in nano-onions can be very important for understanding and predicting other physical properties [17, 18]. Rockenberger *et al.* [8] studied CdTe(core)/CdS(shell) nanoparticles by extended X-ray absorption. They observed changes in the bond lengths of CdTe and CdS, and concluded that small mismatches between the lattice constants of the two materials are elastically compensated by an adjustment of their lattice dimensions in a small interface layer, resulting in a strain. Therefore, they used the classical theory of continuum elasticity to calculate the strain distribution within the core-shell structure by simulating the mismatch strain by a uniform prescribed eigenstrain in the core. For nano-onions, as pointed out by Itskevich *et al.*, Little *et al.*, and Pérez–Conde and Bhattacharjee [17, 19, 20], the misfit strain, the surface stress and the applied external pressure, all modify the strain fields in them, and in turn affect the electronic structures, and hence their physical properties.

The mechanical behaviour of materials at the nanoscale is different from that at the macroscopic scale due to the increased ratio of the surface/interface to the volume. A classical continuum model to explain the surface effect on the elastic properties of nanostructures was formulated by Gurtin and Murdoch [21]. Later, it was further developed by many researchers [22–27] to analyze the elastic properties of nano-structured materials. Miller and Shenoy [22, 25] compared the results obtained by the classical continuum model with those obtained by the atomistic simulations for nanobeams and nanowires, and found that the two methods led almost to the same results. Since a nanostructure can be regarded as a combination of bulk and surface [25], the mechanical behaviour of a nano-structured material can be predicted within the framework of continuum elasticity supplemented by surface elasticity [22, 25, 28]. In fact, Yakobson and Smalley [29] have noted that the laws of continuum mechanics are amazingly robust and allow one to treat even intrinsically discrete objects only a few atoms in diameter.

Core-shell structures also exist widely in conventional particle-reinforced composites and nanocomposites [30–32]. Therefore, the analysis of the stress/strain fields in these particles has also attracted the attention of the researchers in mechanics and composites. Some solutions of elastostatic, viscoelastic and elasto-

plastic problems have been reported [33–38]. However, almost all the existing works on multi-shell models are concerned with the solutions of stress fields under special loading conditions or with the predictions of the effective elastic moduli using approximate schemes.

Recently, DUAN *et al.* [39] have solved the elastostatic problem for a spherical particle with a single graded (with non-homogeneous elastic moduli) shell due to the homogeneous eigenstrains within the Eshelby formalism [40, 41]. DUAN *et al.* [42] analyzed the strain fields in embedded and free-standing nano-onions with multi-shell structure and non-uniform compositions which induce non-uniform eigenstrains. Moreover, they presented a concept of compatible composition profiles and analyzed critical sizes of quantum dots with non-uniform compositions [43]. However, from the point of view of Eshelby formalism, they extended the formalism to multi-shell inhomogeneity or non-uniform inhomogeneity with hydrostatic eigenstrains only [42, 43]. In this paper, we shall use the displacement potential method to solve the elastostatic problems of particles with non-uniform compositions and multi-shells due to arbitrary (uniform or non-uniform) eigenstrains or exterior loadings in the framework of the Eshelby formalism.

The paper is organized as follows. In Sec. 2, we describe the problem under consideration. In Sec. 3, we present the solution for a multi-shell spherical *inhomogeneous inclusion*, namely, a spherical inhomogeneity with multi-shells having different elastic constants subjected to arbitrary uniform eigenstrains in the inhomogeneity and multi-shells. For this problem, the Eshelby tensors are given in concise closed-forms, and the properties of the local and volume average Eshelby tensors are discussed. In Sec. 4, the Eshelby tensors in a finite domain with fixed displacement or traction-free boundary conditions are given. In Sec. 5, we solve the stress field in an infinite medium containing a multi-shell spherical inhomogeneity subjected to an arbitrary uniform remote stress. In this case, we no longer talk about Eshelby tensors but instead introduce stress concentration tensors which relate the stress fields in the inhomogeneity, the multi-shells and the matrix to the remote stress. Finally, in Sec. 6, the Eshelby tensor of a spherical inhomogeneity with non-uniform eigenstrain is obtained and applied to quantum dots with uniform and non-uniform compositions.

## 2. Multi-shell inhomogeneity in an infinite medium

Consider a spherical particle with multi-shells embedded in an infinite elastic matrix, as shown in Fig. 1. Let phase 1 denote the innermost core, hereinafter referred to as the inhomogeneity, and let phase $I$ refer to the shell bounded by the concentric and spherical surfaces with radii $r_I$ and $r_{I+1}$ $(I \in (1, M))$, respectively. Let $\Omega_1$, $\Omega_k\,(k = 2, ...I, ..., M)$ and $\Omega_{M+1}$ denote regions occupied by the inhomogeneity, the multi-shells and the matrix, respectively. The sub-

scripts $k\,(k = 1, 2, ...I, ..., M, M+1)$ are used to denote the quantities in the regions $\Omega_k\,(k = 1, 2, ...I, ..., M, M+1)$. The inhomogeneity, the multi-shells and the matrix are homogeneous, linearly elastic and isotropic, characterized by the bulk modulus $\kappa_k$, the shear modulus $\mu_k$ and the Poisson ratio $\nu_k$ $(k = 1, 2, ...I, ..., M, M+1)$.

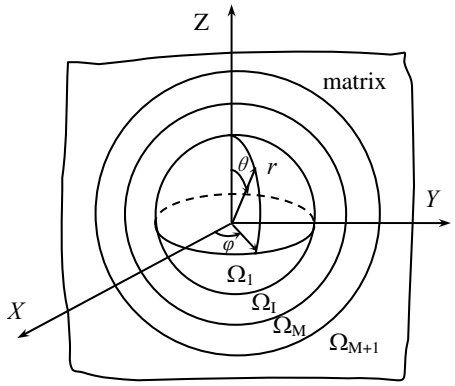


FIG. 1. A spherical inhomogeneity with multi-shells embedded in an infinite medium.

We shall first consider the *inhomogeneous inclusion* problem, namely, when uniform eigenstrains $\boldsymbol{\varepsilon}_I^*$ $(I = 1, 2, ..., M)$ are prescribed in the inhomogeneity and the multi-shells. For this problem, the Eshelby tensors $\mathbf{S}_I^k(\mathbf{x})$ relate the total strains $\boldsymbol{\varepsilon}^k(\mathbf{x})$ in the inhomogeneity $(k = 1)$, the multi-shells $(k = 2, 3, ...M)$, and the matrix $(k = M+1)$ to the prescribed uniform eigenstrains $\boldsymbol{\varepsilon}_I^*$, i.e.,

$$\boldsymbol{\varepsilon}^k = \mathbf{S}_I^k : \boldsymbol{\varepsilon}_I^* + \mathbf{H}^k(\boldsymbol{\sigma}_0^s) \qquad (k = 1, 2, \cdots, M+1), \tag{2.1}$$

where $\mathbf{S}_I^k$ is the Eshelby tensor in the $k$th phase, which relates the uniform eigenstrains $\boldsymbol{\varepsilon}_I^*$ prescribed in the $I$th phase to the strains induced in the $k$th phase. Thus the repeated subscript $I$ in Eq. (2.1) indicates summation from 1 to $M$. $\mathbf{H}^k(\boldsymbol{\sigma}_0^s)$ are the strains due to the constant interface stress $\boldsymbol{\sigma}_0^s$, which will be described below.

The displacement field $\mathbf{u}_I^*$ corresponding to the uniform eigenstrains $\boldsymbol{\varepsilon}_I^*$ in the $I$th phase is expressed as

$$\mathbf{u}_I^* = \boldsymbol{\varepsilon}_I^* \cdot \mathbf{x}, \tag{2.2}$$

where $\mathbf{x}$ is the position vector. As stated in Sec. 1, the large ratio of surface/interface atoms to the bulk can have a profound effect on the properties of nanostructures, and this effect can be described by the classical continuum

model with consideration of the interface effect. Therefore, the interface conditions for this *inhomogeneous inclusion* problem are

$$\begin{aligned} &\mathbf{u}_I + \boldsymbol{\varepsilon}_I^* \cdot \mathbf{x} = \mathbf{u}_{I+1} + \boldsymbol{\varepsilon}_{I+1}^* \cdot \mathbf{x}, \qquad (\boldsymbol{\sigma}_I - \boldsymbol{\sigma}_{I+1}) \cdot \mathbf{N} = \nabla_S \cdot \boldsymbol{\sigma}^s, \\ &\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{at} \quad r = r_{I+1} \\ &\mathbf{u}_{M+1} = \mathbf{0}, \qquad \boldsymbol{\sigma}_{M+1} = \mathbf{0} \qquad \text{at} \quad |\mathbf{x}| \to +\infty, \end{aligned} \tag{2.3}$$

where $\mathbf{N}$ is the unit normal vector to the interface between the $I$th and $(I+1)$th phases, $\nabla_S \cdot \boldsymbol{\sigma}^s$ denotes the interface divergence of the interface stress tensor $\boldsymbol{\sigma}^s$. The interface stress $\boldsymbol{\sigma}^s$ depends on the state of the elastic strain $\boldsymbol{\varepsilon}^s$ [22, 23, 44, 45] and can be expressed as [22]

$$\boldsymbol{\sigma}^s = \boldsymbol{\sigma}_0^s + \mathbf{C}^s : \boldsymbol{\varepsilon}^s, \tag{2.4}$$

where $\mathbf{C}^s$ is the interface modulus tensor. For an elastically isotropic surface/interface, $\mathbf{C}^s : \boldsymbol{\varepsilon}^s = 2\mu_s \boldsymbol{\varepsilon}^s + \lambda_s (\mathrm{tr}\boldsymbol{\varepsilon}^s)\mathbf{1}$, where $\lambda_s$ and $\mu_s$ are the interface moduli, and $\mathbf{1}$ is the second-order unit tensor in two-dimensional space.

We shall next consider the problem when the infinite elastic matrix containing the spherical inhomogeneity with the multi-shells in Fig. 1 is subjected to an arbitrary uniform remote stress field $\boldsymbol{\sigma}^0$. In this case, the stress concentration tensors $\mathbf{T}^k(\mathbf{x})$ $(k = 1, 2, ..., M+1)$ relate the total stresses $\boldsymbol{\sigma}^k(\mathbf{x})$ in the inhomogeneity, the multi-shells and the matrix to the prescribed uniform remote stress $\boldsymbol{\sigma}^0$, i.e.,

$$\boldsymbol{\sigma}^k(\mathbf{x}) = \mathbf{T}^k(\mathbf{x}) : \boldsymbol{\sigma}^0 + \boldsymbol{\sigma}(\boldsymbol{\sigma}_0^s) \quad (k = 1, 2, ..., M+1), \tag{2.5}$$

where $\boldsymbol{\sigma}(\boldsymbol{\sigma}_0^s)$ is the stress tensor due to the constant interface stress tensor $\boldsymbol{\sigma}_0^s$. The interface and boundary conditions for this problem are

$$\begin{aligned} &\mathbf{u}_I = \mathbf{u}_{I+1}, \qquad (\boldsymbol{\sigma}_I - \boldsymbol{\sigma}_{I+1}) \cdot \mathbf{N} = \nabla_S \cdot \boldsymbol{\sigma}^s, \quad \text{at} \quad r = r_{I+1}, \\ &\boldsymbol{\sigma}_{M+1} = \boldsymbol{\sigma}^0 \quad \text{at} \quad |\mathbf{x}| \to +\infty. \end{aligned} \tag{2.6}$$

## 3. Solution of spherical *inhomogeneous inclusion* problem

### 3.1. Solution procedure

The above-mentioned *inhomogeneous inclusion* problem under arbitrary uniform eigenstrains $\boldsymbol{\varepsilon}_I^*$ $(I \in (1, M))$ is solved using the principle of superposition, that is, we obtain the complete set of the components of the Eshelby tensors $\mathbf{S}_I^k(\mathbf{x})$ through the consideration of several particular eigenstrains. For this, we first solve the elastic field induced by $\varepsilon_{zzI}^*$ in the spherical coordinate system $(r, \theta, \varphi)$. The axisymmetric elasticity problem for spherical domains can be solved

in a general fashion in terms of functions of $r$ multiplied by Legendre polynomials of $\theta$. For the present problem, only a solution associated with Legendre polynomials $n = 0, 2$ is needed [46]. It is expedient to split the displacement field into its dilatational part

$$u_r^k = F_{zz}^k r + \frac{G_{zz}^k}{r^2}, \quad u_\theta^k = u_\varphi^k = 0 \tag{3.1}$$

and its deviatoric part

$$u_r^k = U_r^k P_2(\cos\theta), \quad u_\theta^k = U_\theta^k \frac{dP_2(\cos\theta)}{d\theta}, \quad u_\varphi^k = 0 \tag{3.2}$$

in which

$$U_r^k(r) = \left[12\nu_k A_{zz}^k r^3 + 2B_{zz}^k r + \frac{2(5-4\nu_k)C_{zz}^k}{r^2} - 3\frac{D_{zz}^k}{r^4}\right], \tag{3.3}$$

$$U_\theta^k(r) = \left[(7-4\nu_k)A_{zz}^k r^3 + B_{zz}^k r + \frac{2(1-2\nu_k)C_{zz}^k}{r^2} + \frac{D_{zz}^k}{r^4}\right], \tag{3.4}$$

where $P_2(\cos\theta)$ is the Legendre polynomial of order two. $A_{zz}^k$, $B_{zz}^k$, $C_{zz}^k$, $D_{zz}^k$, $F_{zz}^k$ and $G_{zz}^k$ are constants to be determined. The subscript $zz$ of these constants indicates that they are solved for the eigenstrain $\varepsilon_{zzI}^* \neq 0$. For the *inhomogeneous inclusion* problem, these constants are determined from the condition to avoid a singularity at $r = 0$ inside the inhomogeneity and Eq. (2.3). In the inhomogeneity ($k = 1$) $C_{zz}^1, D_{zz}^1$ and $G_{zz}^1$ vanish; in the matrix ($k = M+1$) $A_{zz}^{M+1}, B_{zz}^{M+1}$ and $F_{zz}^{M+1}$ vanish.

Due to the spherical shape of the inhomogeneity and linear property of the problem, the solution due to arbitrary uniform eigenstrains $\boldsymbol{\varepsilon}_I^*$ can be obtained from Eqs. (3.1)–(3.4) by superimposing the individual solutions for $\varepsilon_{xxI}^*$, $\varepsilon_{yyI}^*$, $\varepsilon_{zzI}^*$, $\varepsilon_{xyI}^*$, $\varepsilon_{xzI}^*$ and $\varepsilon_{yzI}^*$, respectively. The detailed procedures of the superposition can be found in the recent paper of DUAN *et al.* [26]. It is found that under $\varepsilon_{xxI}^*, \varepsilon_{yyI}^*, \varepsilon_{zzI}^*, \varepsilon_{xyI}^*, \varepsilon_{xzI}^*$ and $\varepsilon_{yzI}^*$, respectively, the constants $A_{pq}^k$ ($p, q = x, y, z$) are equal for each of $k = 1, 2, ..., M+1$, i.e.,

$$\frac{\partial A_{xx}^k}{\partial \varepsilon_{xxI}^*} = \frac{\partial A_{yy}^k}{\partial \varepsilon_{yyI}^*} = \frac{\partial A_{zz}^k}{\partial \varepsilon_{zzI}^*} = \frac{\partial A_{xy}^k}{\partial \varepsilon_{xyI}^*} = \frac{\partial A_{xz}^k}{\partial \varepsilon_{xzI}^*} = \frac{\partial A_{yz}^k}{\partial \varepsilon_{yzI}^*}, \quad (I = 1, 2, \ldots, M). \tag{3.5}$$

The constants $B_{pq}^k$, $C_{pq}^k$, $D_{pq}^k$, $F_{pq}^k$ and $G_{pq}^k$ also obey their own respective identities. Therefore, for brevity, we introduce constants $A_I^k$, $B_I^k$, $C_I^k$, $D_I^k$, $F_I^k$

and $G_I^k$ for the spherical inhomogeneity, the multi-shells and the matrix such that

$$A_I^k \equiv r_1^2 \frac{\partial A_{pq}^k}{\partial \varepsilon_{pqI}^*}, \qquad B_I^k \equiv \frac{\partial B_{pq}^k}{\partial \varepsilon_{pqI}^*}, \qquad C_I^k \equiv \frac{1}{r_1^3} \frac{\partial C_{pq}^k}{\partial \varepsilon_{pqI}^*},$$

(3.6)

$$D_I^k \equiv \frac{1}{r_1^5} \frac{\partial D_{pq}^k}{\partial \varepsilon_{pqI}^*}, \qquad F_I^k \equiv \frac{\partial F_{pp}^k}{\partial \varepsilon_{ppI}^*}, \qquad G_I^k \equiv \frac{1}{r_1^3} \frac{\partial G_{pp}^k}{\partial \varepsilon_{ppI}^*},$$

where the subscript pairs $pq = xx, yy, zz, xy, xz$ and $yz$ denote the eigenstrain cases $\varepsilon_{xxI}^*, \varepsilon_{yyI}^*, \varepsilon_{zzI}^*, \varepsilon_{xyI}^*, \varepsilon_{xzI}^*$ and $\varepsilon_{yzI}^*$, respectively. Thus, the repeated subscripts in Eq. (3.6) do not represent summation. Note that the last two expressions in Eq. (3.6) are applicable to $pp = xx, yy$ and $zz$ only. The superscript $k$ denotes the $k$-th phase, and $I$ denotes the quantities corresponding to the different eigenstrains. Therefore, the total strain fields in the inhomogeneity and the matrix are expressed in terms of the constants $A_I^k$, $B_I^k$, $C_I^k$, $D_I^k$, $F_I^k$ and $G_I^k$. Knowing these constants, the Eshelby tensors in the *inhomogeneous inclusion*, the multi-shells and matrix can be calculated from the formulae given in the next section, where we shall also discuss their general properties.

### 3.2. Eshelby tensors

Because of the geometrical and physical symmetry of the problem under consideration, the Eshelby tensors in the inhomogeneity and multi-shells are all transversely isotropic tensors with any of the radii being an axis of symmetry. However, it should be noted that unlike the classical Eshelby tensor for an ellipsoidal inhomogeneity without shells, these Eshelby tensors are generally position-dependent. Eshelby tensors are also position-dependent for nano-inhomogeneities because of the interface stress [26]. Using the WALPOLE notation – [47] for transversely isotropic tensors, a fourth-order tensor $\mathbf{S}_I^k(\mathbf{r})$ with the above mentioned radial symmetry can be expressed as

$$\mathbf{S}_I^k(\mathbf{r}) = s_{I1}^k(r)\mathbf{E}^1 + s_{I2}^k(r)\mathbf{E}^2 + s_{I3}^k(r)\mathbf{E}^3 + s_{I4}^k(r)\mathbf{E}^4 + s_{I5}^k(r)\mathbf{E}^5 + s_{I6}^k(r)\mathbf{E}^6 \tag{3.7}$$

or in a concise matrix form

$$\mathbf{S}_I^k(\mathbf{r}) = \widetilde{\mathbf{S}}_I^k(r) \cdot \widetilde{\mathbf{E}}^T \tag{3.8}$$

in which

$$\widetilde{\mathbf{S}}_I^k(r) = \left[\, s_{I1}^k(r) \quad s_{I2}^k(r) \quad s_{I3}^k(r) \quad s_{I4}^k(r) \quad s_{I5}^k(r) \quad s_{I6}^k(r) \,\right], \tag{3.9}$$

$$\widetilde{\mathbf{E}} = \left[ \begin{array}{cccccc} \mathbf{E}^1 & \mathbf{E}^2 & \mathbf{E}^3 & \mathbf{E}^4 & \mathbf{E}^5 & \mathbf{E}^6 \end{array} \right], \tag{3.10}$$

where $\mathbf{r}$ ($\mathbf{r} = r\mathbf{n}$) is the position vector. $\mathbf{n} = n_i\mathbf{e}_i$ is the unit vector along the radius passing the material point at which the Eshelby tensor is calculated, and $r$ is the distance between this point and the origin (the centre of the spherical inhomogeneity). $n_i$ are the direction cosines of $\mathbf{r}$ and $i = 1, 2, 3$ denote $x$-, $y$- and $z$-directions, respectively. $s^k_{Ip}(r)$ ($p = 1, 2, \ldots, 6$) are functions of $r$, and $\mathbf{E}^p$ ($p = 1, 2, \ldots, 6$) are the six elementary tensors introduced by WALPOLE [47].

From the above elastic solutions, the Eshelby tensor in the inhomogeneity is given by Eq. (3.8) with $\widetilde{\mathbf{S}}^1_I(r)$ being

$$\widetilde{\mathbf{S}}^1_I(r) = \left[ \begin{array}{c} \delta_{I1} + B^1_I + 2F^1_I + 3(7 - 8\nu_1)A^1_I\rho^2 \\ \delta_{I1} + 2B^1_I + F^1_I + 36\nu_1 A^1_I\rho^2 \\ \delta_{I1} + 3B^1_I + 3(7 - 4\nu_1)A^1_I\rho^2 \\ \delta_{I1} + 3B^1_I + 3(7 + 2\nu_1)A^1_I\rho^2 \\ -B^1_I + F^1_I - 18\nu_1 A^1_I\rho^2 \\ -B^1_I + F^1_I - 3(7 - 8\nu_1)A^1_I\rho^2 \end{array} \right]^T \tag{3.11}$$

where $\rho = r/r_1$, and the constants $A^1_I, B^1_I$ and $F^1_I$ are given in Eq. (3.6). In the infinite matrix, $\widetilde{\mathbf{S}}^{M+1}_I(r)$ is

$$\widetilde{\mathbf{S}}^{M+1}_I(r) = \left[ \begin{array}{c} 6D^{M+1}_I \dfrac{1}{\rho^5} + 2\left[G^{M+1}_I - 2(1 + \nu_{M+1})C^{M+1}_I\right]\dfrac{1}{\rho^3} \\ 12D^{M+1}_I \dfrac{1}{\rho^5} - 2\left[G^{M+1}_I + 2(5 - 4\nu_{M+1})C^{M+1}_I\right]\dfrac{1}{\rho^3} \\ 3D^{M+1}_I \dfrac{1}{\rho^5} + 6(1 - 2\nu_{M+1})C^{M+1}_I \dfrac{1}{\rho^3} \\ -12D^{M+1}_I \dfrac{1}{\rho^5} + 6(1 + \nu_{M+1})C^{M+1}_I \dfrac{1}{\rho^3} \\ -6D^{M+1}_I \dfrac{1}{\rho^5} - 2\left[G^{M+1}_I - (5 - 4\nu_{M+1})C^{M+1}_I\right]\dfrac{1}{\rho^3} \\ -6D^{M+1}_I \dfrac{1}{\rho^5} + \left[G^{M+1}_I + 4(1 + \nu_{M+1})C^{M+1}_I\right]\dfrac{1}{\rho^3} \end{array} \right]^T \tag{3.12}$$

where the constants $C^{M+1}_I, D^{M+1}_I$ and $G^{M+1}_I$ are given in Eq. (3.6). In the multi-shells, $\widetilde{\mathbf{S}}^k_I(r)$ ($k = 2, ..., M$) is given by

$$
\widetilde{\mathbf{S}}_I^k(r) = \begin{bmatrix}
\delta_{Ik} + B_I^k + 2F_I^k + 3(7-8\nu_k)A_I^k\rho^2 + \dfrac{2}{\rho^3}\left[G_I^k - 2(1+\nu_k)C_I^k\right] + \dfrac{6D_I^k}{\rho^5} \\
\delta_{Ik} + 2B_I^k + F_I^k + 36\nu_k A_I^k\rho^2 - \dfrac{2}{\rho^3}\left[G_I^k + 2(5-4\nu_k)C_I^k\right] + \dfrac{12D_I^k}{\rho^5} \\
\delta_{Ik} + 3B_I^k + 3(7-4\nu_k)A_I^k\rho^2 + 6(1-2\nu_k)C_I^k\dfrac{1}{\rho^3} + 3D_I^k\dfrac{1}{r^5} \\
\delta_{Ik} + 3B_I^k + 3(7+2\nu_k)A_I^k\rho^2 + 6(1+\nu_k)\dfrac{C_I^k}{\rho^3} - \dfrac{12D_I^k}{\rho^5} \\
-B_I^k + F_I^k - 18\nu_k A_I^k\rho^2 - \dfrac{2}{\rho^3}\left[G_I^k - (5-4\nu_k)C_I^k\right] - \dfrac{6D_I^k}{\rho^5} \\
-B_I^k + F_I^k - 3(7-8\nu_k)A_I^k\rho^2 + \left[G_I^k + 4(1+\nu_k)C_I^k\right]\dfrac{1}{\rho^3} - \dfrac{6D_I^k}{\rho^5}
\end{bmatrix}^T \tag{3.13}
$$

If the inhomogeneity, the multi-shells and the matrix have the same elastic moduli, the Eshelby tensors given in Eqs. (3.11) and (3.12) reduce to the classical interior and exterior Eshelby tensors [40].

DUAN *et al.* [39] have shown that the volume average Eshelby tensors can be used to predict the effective elastic moduli of composites. We therefore give the volume averages of the Eshelby tensors for the spherical inhomogeneity with multi-shells. Performing the volume integrations, it is found that the volume average of the Eshelby tensor $\bar{\mathbf{S}}_I^k$ is an isotropic tensor, which can be expressed as

$$
\bar{\mathbf{S}}_I^k = \frac{1}{V_k}\int_{V_k} \widetilde{\mathbf{S}}_I^k(r)\cdot\widetilde{\mathbf{E}}^T\, dV = \xi_I^k\mathbf{K}_1 + \varsigma_I^k\mathbf{K}_2 \tag{3.14}
$$

in which

$$
\mathbf{K}_1 = \frac{1}{3}\mathbf{I}^{(2)}\otimes\mathbf{I}^{(2)}, \quad \mathbf{K}_2 = -\frac{1}{3}\mathbf{I}^{(2)}\otimes\mathbf{I}^{(2)} + \mathbf{I}^{(4s)}, \tag{3.15}
$$

where $V_k$ is the volume of the corresponding phase, $\xi_I^k$ and $\varsigma_I^k$ are constants, and $\mathbf{I}^{(2)}$ and $\mathbf{I}^{(4s)}$ are the second- and fourth-order symmetric identity tensors, respectively. When the inhomogeneity, the multi-shells and the matrix have the same elastic constants, Eq. (3.14) for the interior volume-averaged Eshelby tensor reduces to the classical one [40].

## 4. Eshelby tensors in finite domains

In the preceding section, we gave the general form of the Eshelby tensors of a spherical inhomogeneity with multi-shells in an infinite matrix. In this section, we consider a spherical inhomogeneity and multi-shells with prescribed uniform eigenstrains $\boldsymbol{\varepsilon}_I^*$, in a finite domain whose outer boundary is either fixed or traction-free (Figs. 2(a) and (b)). The Eshelby tensors in the inhomogeneity and multi-shells when the outermost shell is fixed can be obtained from

the general solution by letting the elastic moduli of the matrix tend to infinity. Therefore, we do not report the detailed results here. Instead, we give the results when the outermost shell is traction-free because they can be used to analyse the strain state in free-standing nano-onions. Figure 3 shows spherical free-standing nano-onions with ingredient A (shaded area) and ingredient B. These spherical nano-onions consist of cores and concentric multi-shells of nanometer-size. Here, we distinguish the interface stress from the surface stress for the free-standing nano-onions. Generally, the surface stress $\boldsymbol{\tau}$ can also be expressed by the form similar to Eq. (2.4), i.e., $\boldsymbol{\tau} = \tau_0\mathbf{1}+\mathbf{C}^s : \boldsymbol{\varepsilon}^s$, where $\tau_0$ is the constant surface stress.

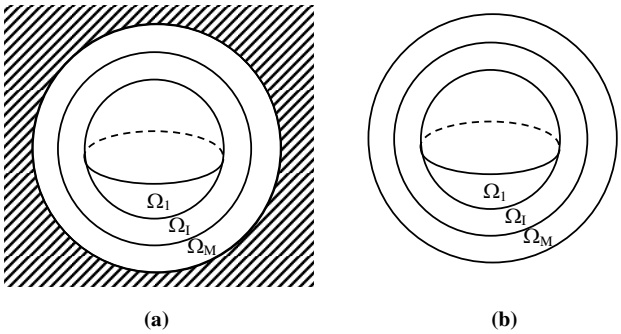


FIG. 2. A spherical inhomogeneity containing multi-shells with fixed exterior boundary (a) and traction-free exterior boundary (b).

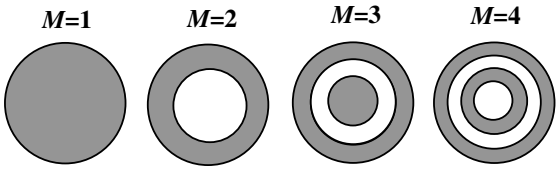


FIG. 3. Spherical free-standing nano-onions with ingredient A (shaded area) and ingredient B.

The interface and boundary conditions for the free-standing nano-onions are

$$\begin{aligned} &\mathbf{u}_I + \boldsymbol{\varepsilon}_I^* \cdot \mathbf{x} = \mathbf{u}_{I+1} + \boldsymbol{\varepsilon}_{I+1}^* \cdot \mathbf{x}, \qquad (\boldsymbol{\sigma}_I - \boldsymbol{\sigma}_{I+1}) \cdot \mathbf{N} = \nabla_S \cdot \boldsymbol{\sigma}^s, \\ &\sigma_{rr} = \frac{2\tau_0}{r_M} \qquad \text{at} \quad r = r_M. \end{aligned} \tag{4.1}$$

It is noted that $\boldsymbol{\varepsilon}_M^* = \mathbf{0}$ and $I \in (1, M-1)$ in Eqs. (2.1) and (4.1) for this traction-free boundary condition. Let us consider a core with two surrounding shells ($M = 3$) as an example to illustrate the procedure. Let the corresponding eigenstrains in the phase 1 and phase 2 be $\boldsymbol{\varepsilon}_1^*$ and $\boldsymbol{\varepsilon}_2^*$, respectively. According to

Eq. (2.1), the total strains in the three phases (1, 2 and 3) are, respectively,

$$
\begin{aligned}
\boldsymbol{\varepsilon}^1 &= \mathbf{S}_1^1 : \boldsymbol{\varepsilon}_1^* + \mathbf{S}_2^1 : \boldsymbol{\varepsilon}_2^* + \mathbf{H}^1(\boldsymbol{\sigma}_0^s, \boldsymbol{\tau}_0) \qquad (\text{in phase } 1),\\
\boldsymbol{\varepsilon}^2 &= \mathbf{S}_1^2 : \boldsymbol{\varepsilon}_1^* + \mathbf{S}_2^2 : \boldsymbol{\varepsilon}_2^* + \mathbf{H}^2(\boldsymbol{\sigma}_0^s, \boldsymbol{\tau}_0) \qquad (\text{in phase } 2),\\
\boldsymbol{\varepsilon}^3 &= \mathbf{S}_1^3 : \boldsymbol{\varepsilon}_1^* + \mathbf{S}_2^3 : \boldsymbol{\varepsilon}_2^* + \mathbf{H}^3(\boldsymbol{\sigma}_0^s, \boldsymbol{\tau}_0) \qquad (\text{in phase } 3),
\end{aligned} \tag{4.2}
$$

where $\mathbf{S}_1^1,\ \mathbf{S}_2^1,\ \mathbf{S}_1^2,\ \mathbf{S}_2^2,\ \mathbf{S}_1^3$ and $\mathbf{S}_2^3$ are six Eshelby tensors in the phases 1, 2 and 3, respectively. The superscripts 1, 2 and 3 denote the quantities corresponding to the phases, and the subscripts 1 and 2 denote the quantities corresponding to eigenstrains $\boldsymbol{\varepsilon}_1^*$ and $\boldsymbol{\varepsilon}_2^*$, respectively. $\mathbf{S}_I^k$ in Eq. (4.2) is given by Eqs. (3.8), (3.11) and (3.13), and the unknown constants in Eqs. (3.11) and (3.13) are determined by the interface and boundary conditions in Eq. (4.1).

## 5. Solution of spherical *inhomogeneity* problem

In the previous two sections, we gave the Eshelby tensors that relate the eigenstrains to the total strains inside the spherical inhomogeneity, the multi-shells and the matrix. In this section, we solve the elastic field of a multi-shell spherical inhomogeneity embedded in an alien matrix which is subjected to a uniform stress $\boldsymbol{\sigma}^0$ at infinity. Because the Eshelby equivalent inclusion method is not used, we shall call the corresponding tensors the stress concentration tensors. These tensors in Eq. (2.5) relate the stress fields in the inhomogeneity, the multi-shells and the matrix to the remote stress tensor $\boldsymbol{\sigma}^0$. As with the *inhomogeneous inclusion* problem in the previous section, the inhomogeneity problem under remote loading is also solved by the principle of superposition [26]. For example, the solutions under $\sigma_{zz}^0$ are still given by Eqs. (3.1)–(3.4) with the constants determined by interface and boundary conditions (2.6) and the condition to avoid a singularity at $r = 0$. In the inhomogeneity ($k = 1$) $C_{zz}^1, D_{zz}^1$ and $G_{zz}^1$ vanish; in the matrix ($k = M + 1$) $A_{zz}^{M+1}$ vanishes, and the remaining constants are determined from the corresponding interface and boundary conditions. It is found that under $\sigma_{xx}^0, \sigma_{yy}^0, \sigma_{zz}^0, \sigma_{xy}^0, \sigma_{xz}^0$ and $\sigma_{yz}^0$, respectively, $A_{pq}^k, B_{pq}^k, C_{pq}^k, D_{pq}^k, F_{pp}^k$ and $G_{pp}^k$ ($p, q = x, y, z$) in the general solutions (3.1)–(3.4) for the inhomogeneity, the multi-shells and the matrix obey relations similar to Eq. (3.5). In this case, we define constants $A^k$, $B^k$, $C^k$, $D^k$, $F^k$ and $G^k$ such that

$$
\begin{aligned}
A^k &\equiv r_1^2 \mu_k \frac{\partial A_{pq}^k}{\partial \sigma_{pq}^0}, \qquad B^k \equiv \mu_k \frac{\partial B_{pq}^k}{\partial \sigma_{pq}^0}, \qquad C^k \equiv \frac{\mu_k}{r_1^3} \frac{\partial C_{pq}^k}{\partial \sigma_{pq}^0},\\
D^k &\equiv \frac{\mu_k}{r_1^5} \frac{\partial D_{pq}^k}{\partial \sigma_{pq}^0}, \qquad F^k \equiv \frac{2(1+\nu_k)}{(1-2\nu_k)} \mu_k \frac{\partial F_{pp}^k}{\partial \sigma_{pp}^0}, \qquad G^k \equiv \frac{\mu_k}{r_1^3} \frac{\partial G_{pp}^k}{\partial \sigma_{pp}^0},
\end{aligned} \tag{5.1}
$$

where the repeated subscripts and superscripts $k$ in Eq. (5.1) do not denote summation.

As before, the subscript pairs $pq = xx, yy, zz, xy, xz$ and $yz$ denote the remote stress cases $\sigma^0_{xx}, \sigma^0_{yy}, \sigma^0_{zz}, \sigma^0_{xy}, \sigma^0_{xz}$ and $\sigma^0_{yz}$, respectively. Again, the last two expressions in Eq. (5.1) are applicable to $pp = xx, yy$ and $zz$ only. Therefore, the total stress fields in the inhomogeneity, the multi-shells and the matrix are expressed in terms of the constants $A^k$, $B^k$, $C^k$, $D^k$, $F^k$ and $G^k$.

The stress concentration tensors of the considered system have the same properties as those of the Eshelby tensors. Therefore, $\mathbf{T}^k(\mathbf{r})$ can be expressed as

$$\mathbf{T}^k(\mathbf{r}) = \widetilde{\mathbf{T}}^k(r) \cdot \widetilde{\mathbf{E}}^T \tag{5.2}$$

where

$$\widetilde{\mathbf{T}}^k(r) = \left[\, T^k_1(r) \quad T^k_2(r) \quad T^k_3(r) \quad T^k_4(r) \quad T^k_5(r) \quad T^k_6(r) \,\right], \tag{5.3}$$

In the inhomogeneity, $\widetilde{\mathbf{T}}^1(r)$ is

$$\widetilde{\mathbf{T}}^1(r) = \begin{bmatrix} 2B^1 + 2F^1 + 6(7+6\nu_1)A^1\rho^2 \\ 4B^1 + F^1 - 12\nu_1 A^1\rho^2 \\ 6B^1 + 6(7-4\nu_1)A^1\rho^2 \\ 6B^1 + 6(7+2\nu_1)A^1\rho^2 \\ -2B^1 + F^1 + 6\nu_1 A^1\rho^2 \\ -2B^1 + F^1 - 6(7+6\nu_1)A^1\rho^2 \end{bmatrix}^T . \tag{5.4}$$

In the matrix, $\widetilde{\mathbf{T}}^{M+1}(r)$ is

$$\widetilde{\mathbf{T}}^{M+1}(r) = \begin{bmatrix} 1 + 12D^{M+1}\dfrac{1}{\rho^5} + 4\left[G^{M+1} - 2(1-2\nu_{M+1})C^{M+1}\right]\dfrac{1}{\rho^3} \\ 1 + 24D^{M+1}\dfrac{1}{\rho^5} - 4\left[G^{M+1} + 2(5-\nu_{M+1})C^{M+1}\right]\dfrac{1}{\rho^3} \\ 1 + 6D^{M+1}\dfrac{1}{\rho^5} + 12(1-2\nu_{M+1})C^{M+1}\dfrac{1}{\rho^3} \\ 1 - 24D^{M+1}\dfrac{1}{\rho^5} + 12(1+\nu_{M+1})C^{M+1}\dfrac{1}{\rho^3} \\ -12D^{M+1}\dfrac{1}{\rho^5} - 4\left[G^{M+1} - (5-\nu_{M+1})C^{M+1}\right]\dfrac{1}{\rho^3} \\ -12D^{M+1}\dfrac{1}{\rho^5} + 2\left[G^{M+1} + 4(1-2\nu_{M+1})C^{M+1}\right]\dfrac{1}{\rho^3} \end{bmatrix}^T \tag{5.5}$$

and in the multi-shells, $\widetilde{\mathbf{T}}^k(r)$ $(k=2,...,M)$ is

$$\widetilde{\mathbf{T}}^k(r)=\begin{bmatrix} 2B^k+2F^k+6(7+6\nu_k)A^k\rho^2+\dfrac{12D^k}{\rho^5}+\dfrac{4}{\rho^3}\left[G^k-2(1-2\nu_k)C^k\right] \\ 4B^k+F^k-12\nu_kA^k\rho^2+\dfrac{24D^k}{\rho^5}-\dfrac{4}{\rho^3}\left[G^k+2(5-\nu_k)C^k\right] \\ 6B^k+6(7-4\nu_k)A^k\rho^2+\dfrac{6D^k}{\rho^5}+12(1-2\nu_k)\dfrac{C^k}{\rho^3} \\ 6B^k+6(7+2\nu_k)A^k\rho^2-\dfrac{24D^k}{\rho^5}+12(1+\nu_k)\dfrac{C^k}{\rho^3} \\ -2B^k+F^k+6\nu_kA^k\rho^2-\dfrac{12D^k}{\rho^5}-\dfrac{4}{\rho^3}\left[G^k-(5-\nu_k)C^k\right] \\ -2B^k+F^k-6(7+6\nu_k)A^k\rho^2-\dfrac{12D^k}{\rho^5}+\dfrac{2}{\rho^3}\left[G^k+4(1-2\nu_k)C^k\right] \end{bmatrix}^T. \tag{5.6}$$

The volume averages of the stress concentration tensors are frequently needed in micromechanical approaches. Performing the volume integrations, it is found that the volume average of the stress concentration tensor is an isotropic tensor, which can be expressed as

$$\bar{\mathbf{T}}^k=\frac{1}{V_k}\int_{V_k}\widetilde{\mathbf{T}}^k(r)\cdot\widetilde{\mathbf{E}}^T dV=\alpha^k\mathbf{K}_1+\beta^k\mathbf{K}_2 \tag{5.7}$$

where $\alpha^k$ and $\beta^k$ are two constants. When the multi-shells and the matrix have the same elastic constants, Eq. (5.7) for the interior stress concentration tensor reduces to the classical one for an inhomogeneity without shells embedded in an alien infinite matrix.

## 6. Eshelby tensors for non-uniform inhomogeneities

In the following, we assume that a spherical inhomogeneity has a spherically symmetric composition, i.e. the non-uniform composition is a function of the radial coordinate $r$ only. Such a nano-inhomogeneity is an appropriate model for solving the strain fields in quantum dots of non-uniform composition, as will be done later in this section. According to VEGARD'S law [48], the non-uniform eigenstrains can be expressed as $\boldsymbol{\varepsilon}^*(r)=x(r)\boldsymbol{\varepsilon}_0^*$, where $\boldsymbol{\varepsilon}_0^*$ is a constant tensor [42]. The existence of the non-uniform eigenstrains will cause an elastic field in a free-standing particle, even when the surface of the particle is not constrained. Thus, in an attempt to find out the elastic fields in the inhomogeneity and matrix, we need to solve first the elastic field in a free-standing inhomogeneity. According to the theory of elasticity, the governing equation to obtain $\mathbf{u}^*$ is as follows:

$$C_{ijkl}\left(u^*_{k,lj}-\varepsilon^*_{kl,j}\right)=0, \tag{6.1}$$

where $C_{ijkl}$ is the elastic moduli tensor of the inhomogeneity and $\varepsilon^*_{ij}$ is the non-uniform eigenstrain. Next, in order to obtain simple analytical solutions, we assume that the elastic moduli of the non-uniform inhomogeneity are constant, i.e., for example the elastic moduli of the $\mathrm{In_xGa_{1-x}As}$ inhomogeneity are those of InAs, and the elastic moduli of the $\mathrm{CdTe_xSe_{1-x}}$ inhomogeneity are those of CdTe. This is a reasonable assumption because the compounds in the inhomogeneity have usually nearly identical elastic constants. First, we consider the elastic fields due to the only non-vanishing $\varepsilon^*_{zz}(r) = x(r)\varepsilon^*_{zz0}$. According to Eqs. (3.1) and (3.2) in Sec. 3, we assume that

$$u^*_r = U_1(r)P_2(\cos\theta) + U_2(r), \qquad u^*_\theta = V_1(r)\frac{dP_2(\cos\theta)}{d\theta}, \qquad u^*_\varphi = 0. \tag{6.2}$$

Substitution of Eq. (6.2) into Eq. (6.1) gives

$$\begin{aligned}
&3(1-\nu_1)\left(r^2\frac{\partial^2 U_2}{\partial r^2} + 2r\frac{\partial U_2}{\partial r}\right) - 6(1-\nu_1)U_2 - \varepsilon^*_{zz0}r^2(1+\nu_1)\frac{\partial x}{\partial r} = 0,\\
&3(1-\nu_1)\left(r^2\frac{\partial^2 U_1}{\partial r^2} + 2r\frac{\partial U_1}{\partial r}\right) - 3(5-8\nu_1)U_1 - 9r\frac{\partial V_1}{\partial r}\\
&\qquad -9(3-4\nu_1)V_1 - 2\varepsilon^*_{zz0}r^2(1-2\nu_1)\frac{\partial x}{\partial r} = 0,\\
&3r\frac{\partial U_1}{\partial r} + 12(1-\nu_1)U_1 + 3(1-2\nu_1)\left(2r\frac{\partial V_1}{\partial r} + r^2\frac{\partial^2 V_1}{\partial r^2}\right)\\
&\qquad - 36(1-\nu_1)V_1 - 2\varepsilon^*_{zz0}r^2(1-2\nu_1)\frac{\partial x}{\partial r} = 0.
\end{aligned} \tag{6.3}$$

For a given variation of $x(r)$, e.g., a linear, logarithmic or exponential variation with $r$, $U_1$, $U_2$ and $V_1$ can be easily determined. In particular, if $x(r)$ in Eq. (6.) is assumed to be a linear function in the radial co-ordinate $r$

$$x(r) = \alpha_0 + \alpha_1\frac{r}{r_1} \tag{6.4}$$

where $\alpha_0$ and $\alpha_1$ are two constants, and $r_1$ denotes the radius of the non-uniform inhomogeneity, then the corresponding $U_1$, $U_2$ and $V_1$ are given as

$$U_1 = \left[12\nu_1 a^1_{zz}r^3 + 2b^1_{zz}r + \frac{2(5-4\nu_1)c^1_{zz}}{r^2} - 3\frac{d^1_{zz}}{r^4}\right] + \frac{r^2\alpha_1\varepsilon^*_{zz0}(3-4\nu_1)}{12r_1(1-\nu_1)}, \tag{6.5}$$

$$U_2 = f^1_{zz}r + \frac{g^1_{zz}}{r^2} + \frac{r^2\alpha_1\varepsilon^*_{zz0}(1+\nu_1)}{12r_1(1-\nu_1)} \tag{6.6}$$

$$V_1 = \left[(7-4\nu_1)a^1_{zz}r^3 + b^1_{zz}r + \frac{2(1-2\nu_1)c^1_{zz}}{r^2} + \frac{d^1_{zz}}{r^4}\right] + \frac{r^2\alpha_1\varepsilon^*_{zz0}(5-6\nu_1)}{36r_1(1-\nu_1)}, \tag{6.7}$$

The constants $a^1_{zz}, b^1_{zz}, c^1_{zz}, d^1_{zz}, f^1_{zz}$ and $g^1_{zz}$ are determined from the traction-free condition at the outer boundary of the free inhomogeneity, and the condition to avoid the singularity at the origin, and are equal to

$$\begin{aligned} a^1_{zz} &= \frac{\alpha_1\varepsilon^*_{zz0}}{18r_1^2(1-\nu_1)(7+5\nu_1)}, \qquad b^1_{zz} = \frac{\alpha_0\varepsilon^*_{zz0}}{3} + \frac{\alpha_1\varepsilon^*_{zz0}(7-5\nu_1^2)}{12(1-\nu_1)(7+5\nu_1)}, \\ f^1_{zz} &= \frac{\alpha_0\varepsilon^*_{zz0}}{3} + \frac{\alpha_1\varepsilon^*_{zz0}(1-2\nu_1)}{6(1-\nu_1)}, \qquad c^1_{zz} = d^1_{zz} = g^1_{zz} = 0. \end{aligned} \tag{6.8}$$

It is seen that even when the surface of the particle is not constrained, the non-uniform eigenstrain still causes an elastic stress/strain field in the particle. When the non-uniform inhomogeneity is embedded in an infinite (relative to the inhomogeneity size) or finite alien medium, the constraint imposed by the exterior medium will cause an additional elastic field. It is found that under $\varepsilon^*_{xx0}, \varepsilon^*_{yy0}, \varepsilon^*_{zz0}, \varepsilon^*_{xy0}, \varepsilon^*_{xz0}$ and $\varepsilon^*_{yz0}$, respectively, $c^1_{pq} = d^1_{pq} = g^1_{pp} = 0$ $(p, q = x, y, z)$, and $a^1_{pq}, b^1_{pq}$ and $f^1_{pp}$ $(p, q = x, y, z)$ in the general solutions (6.5)–(6.7) for the inhomogeneity obey relations similar to Eq. (3.5). In this case, we define constants $a^1$, $b^1$ and $f^1$ such that

$$a^1 \equiv r_1^2\frac{\partial a^1_{pq}}{\partial\varepsilon^*_{pq0}}, \quad b^1 \equiv \frac{\partial b^1_{pq}}{\partial\varepsilon^*_{pq0}}, \quad f^1 \equiv \frac{\partial f^1_{pp}}{\partial\varepsilon^*_{pp0}}, \tag{6.9}$$

where the subscript pairs $pq = xx, yy, zz, xy, xz$ and $yz$ denote the eigenstrain cases $\varepsilon^*_{xx0}, \varepsilon^*_{yy0}, \varepsilon^*_{zz0}, \varepsilon^*_{xy0}, \varepsilon^*_{xz0}$ and $\varepsilon^*_{yz0}$, respectively.

In what follows, we will calculate the elastic field by embedding the non-uniform inhomogeneity in an infinite medium or a finite shell. For the embedded nano-onion, the displacement fields in the inhomogeneity and the matrix are given by Eqs. (3.1) and (3.2). In the case of inhomogeneity $(k = 1)$ $c^1_{zz}, d^1_{zz}$ and $g^1_{zz}$ vanish; in the matrix $(k = 2)$ $a^2_{zz}, b^2_{zz}$ and $f^2_{zz}$ vanish. The other constants are determined from the following interface conditions:

$$\mathbf{u}^2 = \mathbf{u}^1 + \mathbf{u}^*\,|_{r=r_1}, \quad (\boldsymbol{\sigma}^1 - \boldsymbol{\sigma}^2)\cdot\mathbf{N} = \nabla_S\cdot\boldsymbol{\sigma}^s \tag{6.10}$$

where $\mathbf{u}^1$ is the displacement in the inhomogeneity caused only by the constraint imposed by the matrix, and $\mathbf{u}^2$ is the total displacement in the matrix. The expressions of $\mathbf{u}^1$ and $\mathbf{u}^2$ are the same as those for a spherical inhomogeneity with multi-shell structures.

For the case of non-uniform eigenstrain $\boldsymbol{\varepsilon}^*(r) = \boldsymbol{\varepsilon}^*_0(\alpha_0 + \alpha_1 r/r_1)$, according to the same procedures as those used for the inhomogeneity with multi-shell

structure, we define constants $\mathcal{A}^k$, $\mathcal{B}^k$, $\mathcal{C}^k$, $\mathcal{D}^k$, $\mathcal{F}^k$ and $\mathcal{G}^k$ for the spherical inhomogeneity and the matrix such that

$$\begin{aligned} \mathcal{A}^k &\equiv r_1^2 \frac{\partial \mathcal{A}^k_{pq}}{\partial \varepsilon^*_{pq0}}, \qquad \mathcal{B}^k \equiv \frac{\partial \mathcal{B}^k_{pq}}{\partial \varepsilon^*_{pq0}}, \qquad \mathcal{C}^k \equiv \frac{1}{r_1^3}\frac{\partial \mathcal{C}^k_{pq}}{\partial \varepsilon^*_{pq0}}, \\ \mathcal{D}^k &\equiv \frac{1}{r_1^5}\frac{\partial \mathcal{D}^k_{pq}}{\partial \varepsilon^*_{pq0}}, \qquad \mathcal{F}^k \equiv \frac{\partial \mathcal{F}^k_{pp}}{\partial \varepsilon^*_{pp0}}, \qquad \mathcal{G}^k \equiv \frac{1}{r_1^3}\frac{\partial \mathcal{G}^k_{pp}}{\partial \varepsilon^*_{pp0}}. \end{aligned} \tag{6.11}$$

Therefore, in analogy with Eq. (2.1), we define Eshelby tensors $\mathbf{J}^k(\mathbf{x})$ that relate the total strains $\boldsymbol{\varepsilon}^k(\mathbf{x})$ in the non-uniform inhomogeneity($k = 1$) and the matrix ($k = 2$) to the prescribed eigenstrain

$$\boldsymbol{\varepsilon}^k = \mathbf{J}^k(\mathbf{r}) : \boldsymbol{\varepsilon}^*_0 + \mathbf{H}^k(\boldsymbol{\sigma}^s_0), \tag{6.12}$$

where $\mathbf{J}^k(\mathbf{r})$ is a transversely isotropic tensor

$$\mathbf{J}^k(\mathbf{r}) = \widetilde{\mathbf{J}}^k(r) \cdot \widetilde{\mathbf{E}}^T. \tag{6.13}$$

in which

$$\widetilde{\mathbf{J}}^k(r) = \begin{bmatrix} j^k_1(r) & j^k_2(r) & j^k_3(r) & j^k_4(r) & j^k_5(r) & j^k_6(r) \end{bmatrix}. \tag{6.14}$$

The Eshelby tensor in the inhomogeneity, $\widetilde{\mathbf{J}}^1(r)$ is

$$\widetilde{\mathbf{J}}^1(r) = \begin{bmatrix} \mathcal{B}^1 + b^1 + 2(\mathcal{F}^1 + f^1) + 3(7-8\nu_1)(\mathcal{A}^1 + a^1)\rho^2 + \dfrac{\rho\alpha_1}{3(1-\nu_1)} \\ 2(\mathcal{B}^1 + b^1) + \mathcal{F}^1 + f^1 + 36\nu_1(\mathcal{A}^1 + a^1)\rho^2 + \dfrac{(3-4\nu_1)\rho\alpha_1}{6(1-\nu_1)} \\ 3(\mathcal{B}^1 + b^1) + 3(7-4\nu_1)(\mathcal{A}^1 + a^1)\rho^2 + \dfrac{(5-6\nu_1)\rho\alpha_1}{12(1-\nu_1)} \\ 3(\mathcal{B}^1 + b^1) + 3(7+2\nu_1)(\mathcal{A}^1 + a^1)\rho^2 + \dfrac{(7-9\nu_1)\rho\alpha_1}{12(1-\nu_1)} \\ -\mathcal{B}^1 - b^1 + \mathcal{F}^1 + f^1 - 18\nu_1(A^1 + a^1)\rho^2 - \dfrac{(1-6\nu_1)\rho\alpha_1}{12(1-\nu_1)} \\ -\mathcal{B}^1 - b^1 + \mathcal{F}^1 + f^1 - 3(7-8\nu_1)(\mathcal{A}^1 + a^1)\rho^2 - \dfrac{(1-3\nu_1)\rho\alpha_1}{12(1-\nu_1)} \end{bmatrix}^T \tag{6.15}$$

where $a^1, b^1, f^1$ are given in Eq. (6.9), and $\mathcal{A}^1, \mathcal{B}^1, \mathcal{F}^1$ are given in Eq. (6.11). In the matrix, $\widetilde{\mathbf{J}}^2(r)$ has the same form as Eq. (3.12) with $M = 1$, and $C_I^{M+1}$, $D_I^{M+1}$ and $G_I^{M+1}$ are replaced by $\mathcal{C}^2$, $\mathcal{D}^2$ and $\mathcal{G}^2$, respectively.

## 7. Numerical results

As seen from the above theoretical analysis, interface stress has effect on the elastic fields of the composites containing nanoparticles with multi-shells. To evaluate the influence of interface stress on the elastic fields of this kind of nano-composites, we first study the total stress distribution in the nano-particle with a shell embedded in an infinite matrix, with the effect of interface stress expressed by Eq. (2.4). Here, we assume that the interface constitutive equation is isotropic, i.e., there are two interface parameters $\lambda_s$ and $\mu_s$ on each of the two interfaces. The material and geometric parameters used for the numerical calculations are as follows. The shear moduli are $\mu_3 = 10\text{GPa}$, $\mu_1 = 10\mu_3$ and $\mu_2 = 4\mu_3$ and Poisson's ratios are $\nu_1 = \nu_2 = \nu_3 = 0.3$; the radii of inhomogeneity and shell are $r_1 = 6\text{nm}$, $r_2 = 9\text{nm}$, respectively. The normalized total radial stress $(\sigma_{rr}/\Sigma^0)$ due to $\sigma^0_{xx} = -\sigma^0_{yy} = \Sigma^0$ are shown in Fig. 4. It is noted that previously, HERVE and ZAOUI [33] have solved the elastic field in an infinite medium containing a spherical inhomogeneity with multiple homogeneous shells. For comparison purposes, we have also drawn the results of HERVE and ZAOUI [33] in Fig. 4. It can be seen that the interface parameter has a significant effect on the stress distribution, especially in the nanoparticle. When interface parameters are equal to zero, our results reduce to those of HERVE and ZAOUI [33].

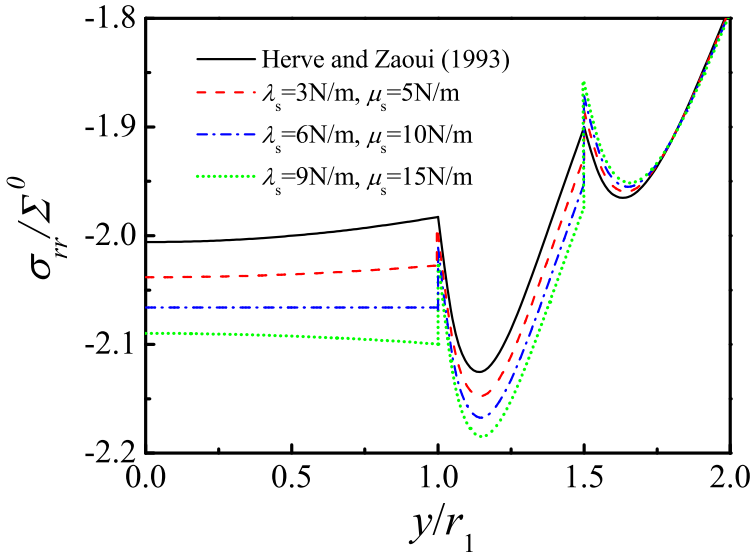


FIG. 4. Stress distribution in a spherical uniform nano-particle with one shell ($M = 2$) embedded in an infinite matrix for different values of interface moduli $\lambda_s$ and $\mu_s$.

Next, let us compare the total strain distribution in the uniform nano-onion with one shell CdS/ZnS ($M = 2$), embedded in an infinite CdS matrix with that

in the non-uniform nano-onion $Zn_xCd_{1-x}S$ embedded in an infinite CdS matrix. It is noted that the elastic moduli of nano-structured quantum dots (QDs) are different from those of bulk materials due to the increased ratio of the surface to the volume. The elastic moduli of nanoparticles (or nanowires and nanofilms, etc.) can be characterized by apparent (or effective) moduli, which reflect the surface effect [25, 28, 49], and a simple scaling law for the properties of nano-structured materials has been given by WANG *et al.* [28]. However, because of the lack of information on the surface properties of QDs under consideration, we cannot determine the exact effective elastic moduli of nano-structured QDs. Therefore, we assume that the elastic moduli of nano-structured QDs are the same as those of the corresponding bulk materials.

The elastic constants of bulk ZnS and CdS are as follows: ZnS, bulk modulus 81.6 GPa, Poisson's ratio 0.4; and CdS, bulk modulus 62.3 GPa, Poisson's ratio 0.4. The lattice constants of ZnS and CdS are $a = 5.409$, $a = 5.815$, respectively. Therefore, the misfit strain due to the mismatch of the lattice constants of ZnS(core)/CdS(shell) is $\varepsilon^*_{m0} = -7.0\%$. We consider the case of $Zn_xCd_{1-x}S$ for which in Eq. (6.4): $\alpha_0 = 1, \alpha_1 = -0.4$, and $r_1 = 9$ nm. For CdS/ZnS/CdS: $r_1 = 6$ nm, $r_2 = 9$ nm. We assume that there exists a constant interface stress $\boldsymbol{\sigma}^s = \sigma^s_0\mathbf{1}$ in CdS/ZnS/CdS and $Zn_xCd_{1-x}S$ QDs and $\sigma^s_0 = 1\text{N/m}$. The normalized total radial strain $(\varepsilon_{rr}/\varepsilon^*_{m0})$ both for CdS/ZnS and $Zn_xCd_{1-x}S$ under $\varepsilon^*_{zz}(r) = x(r)\varepsilon^*_{m0}$, are shown in Figs. 5–6. It can be seen that the distributions of the total radial strains are strongly dependent on the compositions and structures of the nano-onions, and are different for $Zn_xCd_{1-x}S$ and CdS/ZnS $(M = 2)$.

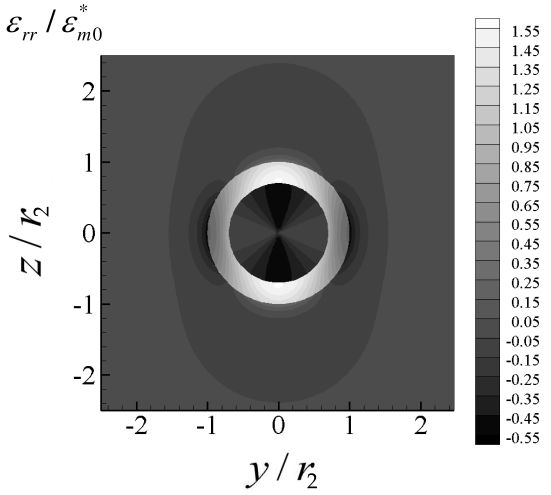


FIG. 5. Strain distribution in a spherical uniform nano-onion with one shell $(M = 2)$ embedded in an infinite matrix with a constant interface stress $\sigma^s_0 = 1\text{N/m}$.

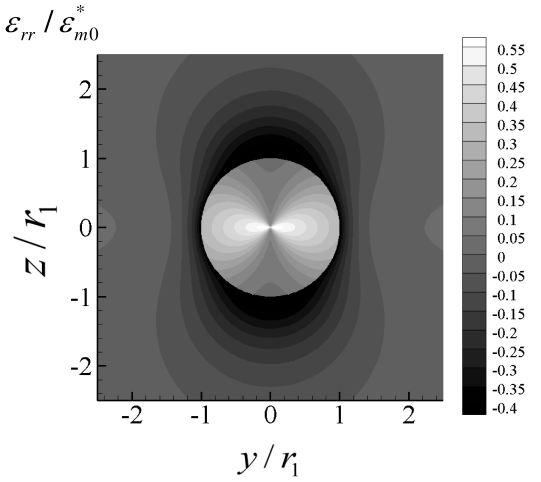


FIG. 6. Strain distribution in a non-uniform spherical QD embedded in an infinite matrix with a constant interface stress $\sigma_0^s = 1\text{N/m}$.

## 8. Concluding remarks

The mechanical behaviour of materials at the nanoscale is different from that at the macroscopic scale due to the increasing ratio of the surface to the volume. Recently, many attempts have been made to reveal the influence of surface properties on the elastic properties of nanobeams, nanowires, nanoplates, etc. The theoretical and experimental works of MILLER and SHENOY [22], JING *et al.* [50] and DUAN *et al.* [26, 27] showed that the elastic moduli of homogeneous and heterogeneous materials varied with their characteristic size due to the surface effect. It can be seen from above, an isotropic surface/interface is characterized by two surface/interface elastic constants $\lambda_s$ and $\mu_s$, giving rise to two intrinsic length scales $l_\lambda = |\lambda_s|/\mu_{M+1}$ and $l_\mu = |\mu_s|/\mu_{M+1}$. Therefore, the Eshelby and stress concentration tensors for the nano-inhomogeneities with muliti-shells are found to depend on these two intrinsic length scales and on the size of the inhomogeneity, i.e. both on relative and absolute sizes.

Based on the theory of the surface elasticity [26], the elastic solutions of the nano-inhomogeneities with arbitrary shape can be obtained by using the same techniques. For example, WANG and WANG [51] obtained the elastic solutions of a nanosized elliptical hole by using the complex variable formulation. LIPIŃSKI *et al.* [52] obtained the elastic solutions of an ellipsoidal multi-coated inclusion by using Green's function techniques. The problems of nano-inhomogeneities with ellipsoidal shape can also be solved by Green's function techniques. This will be investigated in the future. Based on our analysis and the concluding remarks, the following conclusions can be drawn:

1. We have obtained the analytical solutions of the elastostatic *inhomogeneous inclusion* problem of an infinite medium containing a spherical particle with multi-shells when eigenstrains are prescribed in the particle and in the multi-shells, and the *inhomogeneity* problem when an arbitrary remote stress field is prescribed. The corresponding Eshelby and stress concentration tensors are presented.
2. The analytical solutions of inhomogeneous inclusions in finite spherical domains with fixed displacement or traction-free boundary conditions have been obtained.
3. The strain fields in the spherical non-uniform inhomogeneity due to non-uniform eigenstrains have been solved and applied to quantum dots with uniform and non-uniform compositions. The information on the stress fields in embedded core-shell particles can also be used to analyse the damage mechanisms in composites containing these particles.

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