# A curvature-dependent interfacial energy-based interface stress theory and its applications to nano-structured materials: (I) General theory

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ABSTRACT

Experimental observations have shown the size-dependent residual surface stresses on spherical nanoparticles and their influence on the effective modulus of heterogeneous nanostructures. Based on these experimental findings, this paper proposes a new interface stress theory that considers the curvature effect on the interfacial energy. To investigate this curvature-dependent interfacial energy, we use the Green elasticity theory to describe the nonlinear constitutive relation of the interface at finite deformation, thus explicitly demonstrating the curvature-dependent nature of the interface stress and bending moment. By introducing a fictitious stress-free configuration, we then propose a new energy functional for heterogeneous hyperelastic solids with interfaces. For the first time, both the Lagrangian and Eulerian descriptions of the generalized Young–Laplace equation, which describes the intrinsic flexural resistance of the interface, are derived from the newly developed energy functional. This new interface stress theory is then used to investigate the residual elastic field in a heterogeneous hyperelastic solid containing interfaces. The present theory differs from the existing theories in that it takes fully into account both the curvature-dependence of the interfacial energy and the interfacial energy-induced residual elastic field in the bulk solid. Furthermore, the fundamental equations of the interface are given in Lagrangian description, which are preferable when considering the effects of residual interface stress, residual interface bending moment and interface elasticity. Finally, two examples are presented to shed light on the significance of this new interface stress theory. A more detailed analysis and applications of the new theory will be presented in Part (II) of this paper.

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## 1. Introduction

Atoms at surfaces and interfaces experience a different local environment from atoms inside bulk materials, and the physical states and equilibrium positions of such atoms will, generally, differ from those of the interior atoms. This difference is the physical origin of the surface/interfacial energy and the surface/interface stress in solids and liquids, a topic which has been fully studied by many researchers (e.g., Gibbs, 1906; Shuttleworth, 1950; Herring, 1953; Orowan, 1970;

Murr, 1975; Cahn, 1978; Povstenko, 1993; Cammarata, 1994; Weissmuller and Cahn, 1997). In the Gibbsian formulation of the thermodynamics of the surface/interface, the surface/interfacial energy represents the excess free energy due to the existence of a surface/interface and is defined as the reversible work per unit area needed to create a new surface/interface. When the surface/interface of a solid is deformed, the surface/interfacial energy will generally vary. The surface/interface stress is associated with the reversible work per unit area needed to elastically stretch a pre-existing surface/interface. From the above definitions, then it can be seen that the surface/interfacial energy and surface/interface stress have different natures. For liquids, owing to the atomic mobility, the surface atoms increase during stretching since the interior atoms in the liquid can flow freely to the surface of the liquid and therefore the magnitudes of the surface energy and the surface stress (surface tension) are the same. The atomic mobility in solids, by contrast, is very low, and the total amount of the surface atoms remains constant under elastic stretching; thus the surface stress of solids usually varies with deformation. The relationship between the surface stress and the surface strain is given by the famous Shuttleworth–Herring equation (Shuttleworth, 1950; Herring, 1951). As surfaces and interfaces have similar roles in continuum mechanics, we shall, for expediency, use the word "interface" to refer to both of them when describing general principles and when there is no need to differentiate two.

In recent years, tremendous progress has been made in nanotechnology owing to the promise it holds for the engineering applications in micro-electro-mechanical systems and nano-intelligent devices. Research results have increasingly shown that some important physical properties of the nano-structured materials, such as the elastic modulus, melting temperature and yield strength, become size-dependent (Miller and Shenoy, 2000; Sun et al., 2002; Chen et al., 2006; Jing et al., 2006; Zhang et al., 2010). Consequently, determining how to explain these interesting phenomena has been a key goal in mechanics, material science and solid state physics. At the nanoscale, the size-dependent physical properties of materials can be rationalized by invoking the concept of surface/interfacial energy, because the surface/interface-to-volume ratios of the nano-structured materials are so remarkably large that the surface/interface effect must be taken into account.

Any investigation of the surface/interface effect on the heterogeneous nano-structured materials requires a comprehensive surface/interface theory in order to allow for understanding of the physical mechanisms of their fantastic properties and also demonstrates how these are meaningful for engineering applications. A systematic theory describing the mechanical behaviors of the material surfaces of solids was first established by Gurtin and Murdoch (1975, 1978) within the framework of continuum mechanics. In their theory, the constitutive relation and equilibrium equation of the surface are given. This work has been extended by Gurtin and his co-workers to take the thermal effects into account (Angenent and Gurtin, 1989; Gurtin, 1988; Gurtin and Struthers, 1990). With the rapid developments in nanoscience and nanotechnology, the Gurtin–Murdoch theory has been widely used to analyze the size-dependent elastic properties of nanomaterials and nanostructures, including nanowires (Chen et al., 2006; Jing et al., 2006), nanofilms (Cammarata, 1994; Streitz et al., 1994a, 1994b; Dingreville et al., 2005; He et al., 2004), nanovoids (He and Li, 2006) and composites with nano-inhomogeneities (Sharma et al., 2003; Sharma and Ganti, 2004; Duan et al., 2005a,b; Sharma and Wheeler, 2007).

A series of important studies published by Huang's group (Huang and Wang, 2006; Huang and Sun, 2007) showed that residual interface stress induces a residual elastic field in the bulk due to the existence of interfacial energy. Therefore, there exists a non-zero stress field in the bulk for heterogeneous materials containing interfaces even without external load. According to Hoger's work (e.g., Hoger, 1986, 1993), the theory of residually stressed elastic solids dramatically differs from the classical theory of elasticity in that the elastic tensors in the constitutive equations depend explicitly on the residual stress. Based on this physical fact, Huang's group developed an interfacial energy theory for the multi-phase hyperelastic media at finite deformation (Huang and Wang, 2013). In their theory, the Lagrangian description of the interface equilibrium equations is preferred and the first Piola–Kirchhoff interface stress is used in order to correctly deal with the above-mentioned residual elastic field. Their work emphasized the importance of the residual elastic field and concluded that the residual interface stress does have a significant influence on the effective elastic properties of nano-structured materials, something which had been neglected by most previous researchers. Recently, Mi and Kouris (2012)'s work on the interface effects for the embedded nanoparticles demonstrated that the residual interface stress played a more important role in the stress distribution than the interface elasticity. Their work was based on the theory of interface stress developed by Gurtin and Murdoch (1975, 1978), thus did not account for the curvature-dependence of the interfacial energy.

It should be pointed out that the interface theories mentioned above are based on the assumption that the interfacial energy is only relevant to the interface strain, and the residual interface stress in these theories is constant for a given material. However, Tolman (1949) demonstrated the effect of droplet size on the surface tension by employing the Gibbs thermodynamic theory and proposed the venerable Tolman's formula, making the Tolman length a hot area of research to this day (Lei et al., 2005). As a matter of fact, there is an intrinsic flexural resistance of the interface since the interface region has a few atomic layers' thickness. Inspired by the pioneering work of Tolman (1949), one can conclude that the interfacial energy should depend not only on the interface strain but also on the interface curvature.

The curvature-dependence of the interfacial energy was studied by many researchers from the viewpoints of physics and chemistry (Jiang et al., 2001; Lu and Jiang, 2004, 2005; Medasani et al., 2007; Das and Binder, 2011; Nanda, 2012). Their work has shown that the interfacial energy and the interface stress of nanomaterials are generally curvature-dependent and have important applications in physical processes at the nanoscale (Jiang and Lu, 2008). Notably, the curvature-dependence of the surface/interfacial free energy also plays a significant role in the stability and evolution of the configurations of cell membranes (Helfrich, 1973; Ou-Yang and Helfrich, 1987). However, most of the above-mentioned works are mainly concerned with simple nanostructures in their initial natural states and thus use only the classical Tolman length to

characterize the curvature-dependence of the interfacial energy and interface stress. The relationship among the curvature-dependent interfacial energy, the interface stress and the interface deformation under external loads has not been well studied.

Using the theory of elastic shells, Steigmann and Ogden (1999) generalized the Gurtin–Murdoch theory to take into account the effect of flexural resistance of elastic films attached to the bounding surfaces of solids. In their theory, the effect of interface curvature on the interfacial energy is considered. Later, Chhapadia et al. (2011) gave a simplified and linearized version of the Steigmann–Ogden theory to study the influences of the curvature-dependent surface energy on nanostructures. They suggested that in some cases the importance of the curvature dependence of the surface energy should be taken seriously (Mohammadi and Sharma, 2012). However, these interface models ignored the residual elastic field in the bulk induced by the surface/interfacial energy. As emphasized in the literature (Sun et al., 2004; Huang and Sun, 2007), the residual elastic field has a significant impact on the mechanical behaviors of nano-structured materials. This effect has also been confirmed by Park and Klein (2008) in their study of the resonant properties of nanowires.

As the interface region has only a few atomic layers, the interface is usually idealized as a "mathematical interface" with zero thickness in macroscopic continuum descriptions. It should be pointed out that the surface/interface stress models reviewed above belongs to this mathematical interface model. According to the adhering conditions between two different materials, there are also many other types of interface models in the literature to deal with the interface problems in heterogeneous media, including the imperfect interface models such as the linear-spring model (Hashin, 1991a, b; Qu, 1993; Zhong and Meguid, 1997, 1999; Shen et al., 2000), the free sliding model (Ghahremani, 1980; Mura and Furuhashi, 1984; Mura et al., 1985; Huang et al., 1993), the Ramberg–Osgood model (Zhang and Huang, 2004), etc. In this paper, only the interface stress model, in which the displacement is continuous across the interface while the stress undergoes a discontinuity, is considered.

In summary, the curvature-dependence of the interfacial energy and the residual elastic field in the bulk induced by the interfacial energy are two essential features of the material interface in heterogeneous solids, both of which play significant roles in the interface stress model, and neither of which can be ignored. Nevertheless, a more general interface theory considering both of these two effects has not been well developed.

In this study, we develop a new interface stress theory in which both of the above-mentioned effects are taken into account. The key objectives and contributions of this paper are as follows:

1. To explicitly formulate the nonlinear interface constitutive relation at finite deformation based on the interfacial free energy function, which depends on both the in-plane interfacial strain and curvature of the interface;
2. To elucidate in detail the concept of the interfacial energy-induced residual elastic field and its significance;
3. To systematically derive the generalized Young–Laplace equation in both Lagrangeian and Eulerian descriptions using the newly developed energy functional.

Unlike the conventional surface/interface stress theory reported in the current literature, this new theory is capable of predicting the size-dependence of the residual surface stress of spherical nanoparticles, which is in good agreement with the Tolman's formula (Tolman, 1949) and the related calculation results (Medasani and Vasiliev, 2009). Furthermore, a set of basic equations for determining the residual elastic field in the heterogeneous media containing interfaces is provided. The residual elastic field in the hyperelastic media with nanovoids is studied and it is shown that the curvature-dependence of the residual surface stress does have a significant influence on distributions of the residual stresses in the elastic body. Finally, a new dimensionless intrinsic parameter is suggested to estimate the importance of the curvature-dependent part of the residual surface stress.

The outline of this paper is as follows. Section 2 (next) provides a preliminary introduction to the geometry of a deformable interface. Section 3 formulates the nonlinear constitutive relation of the interface at finite deformation. Section 4 is dedicated to the concept of the residual elastic field induced by the interfacial energy. Section 5 shows how the generalized Young–Laplace equation can be systematically derived. Section 6 is concerned with the determination of the residual elastic field in the bulk. Finally, Section 7 provides two examples that illustrate the use of the newly developed theory.

## 2. Deformation and kinematics of the interface

In this section, we will provide some preliminary definitions and notations that are necessary for describing the deformation of an interface. For details, the author may refer to Huang (2012) and Huang and Wang (2013).

### 2.1. Geometric relations at finite deformation

Consider a multi-phase hyperelastic solid containing sharp interfaces between the phases. This configuration is referred to as the initial reference configuration, denoted by $\kappa_0$, when no external load is applied. The interfaces are denoted collectively by $A_0$. A curvilinear coordinate system $\theta^\alpha (\alpha = 1, 2)$ will be used to describe the material point $\boldsymbol{Y}$ on the surface. The corresponding covariant base vectors at point $\boldsymbol{Y}$ in the reference configuration can be determined by $\boldsymbol{A}_\alpha = \boldsymbol{Y}_{,\alpha}$ with $\boldsymbol{A}_3$
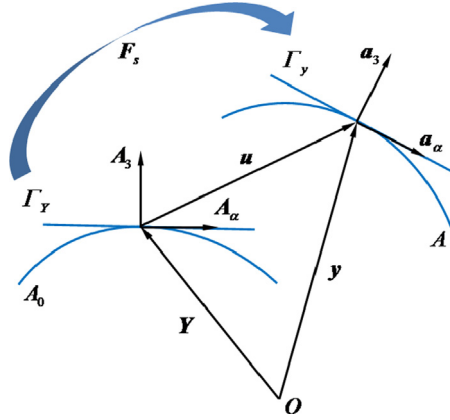
**Fig. 1.** A surface/interface before and after deformation.

being the unit normal vector. Here and in the following, the Greek indices take values in {1, 2}, and the Latin indices take values in {1, 2, 3}.

After deformation, the material point $\boldsymbol{Y}$ on the interface $A_0$ in the reference configuration will move to a point $\boldsymbol{y}$ on the interface $A$ in the current configuration, denoted by $\kappa$. As shown in Fig. 1, the corresponding covariant base vectors at point $\boldsymbol{y}$ on the interface $A$ can be written as $\boldsymbol{a}_\alpha = \boldsymbol{y}_{,\alpha} = \boldsymbol{Y}_{,\alpha} + \boldsymbol{u}_{,\alpha}$ with $\boldsymbol{a}_3$ being the unit normal vector, where $\boldsymbol{u}$ is the displacement. If the displacement $\boldsymbol{u}$ is decomposed into a sum of $\mathbf{u}_{0s} = u_0^\alpha \mathbf{A}_\alpha$ in the tangential direction and $\mathbf{u}_{0n} = u_0^n \mathbf{A}_3$ in the normal direction of the interface $A_0$, then the base vector $\boldsymbol{a}_\alpha$ can be expressed in the reference configuration, which gives

$$\boldsymbol{a}_\alpha = \mathbf{A}_\alpha + \left( u_0^\beta \mathbf{A}_\beta \right)_{,\alpha} + \left( u_0^n \mathbf{A}_3 \right)_{,\alpha} = \mathbf{A}_\alpha + (u_0^\lambda|_\alpha - u_0^n B_\alpha^\lambda)\mathbf{A}_\lambda + \left( u_0^\lambda B_{\lambda\alpha} + u_{0,\alpha}^n \right)\mathbf{A}_3 \tag{1}$$

where "|" denotes covariant derivative and $\mathbf{B} = B_{\lambda\alpha}\mathbf{A}^\lambda \otimes \mathbf{A}^\alpha$ is the curvature tensor of the surface $A_0$. Therefore, the interface deformation gradient can be written as

$$\mathbf{F}_s = \boldsymbol{a}_\alpha \otimes \mathbf{A}^\alpha = \mathbf{F}_s^{(in)} + \mathbf{F}_s^{(ou)} \tag{2}$$

where the in-plane term $\mathbf{F}_s^{(in)}$ and the out-plane term $\mathbf{F}_s^{(ou)}$ are

$$\mathbf{F}_s^{(in)} = \mathbf{i}_0 + \mathbf{u}\nabla_{0s}, \quad \mathbf{F}_s^{(ou)} = \mathbf{A}_3 \otimes \mathbf{D} \tag{3}$$

In the above, $\mathbf{i}_0$ is the unit tensor on surface $A_0$, $\mathbf{u}\nabla_{0s} = \mathbf{u}_{0s}\nabla_{0s} - u_0^n \mathbf{B}$ is the surface displacement gradient and $\mathbf{D} = \mathbf{u}_{0s} \cdot \mathbf{B} + u_0^n \nabla_{0s}$ in the reference configuration.

Similarly, the displacement $\boldsymbol{u}$ can also be decomposed as the sum of its tangential component $\mathbf{u}_s = u^\alpha \boldsymbol{a}_\alpha$ and normal component $\mathbf{u}_n = u^n \boldsymbol{a}_3$ on the interface $A$, then the base vectors $\mathbf{A}_\alpha$ can be expressed in the current configuration, which gives

$$\mathbf{A}_\alpha = \boldsymbol{a}_\alpha - (u^\beta \boldsymbol{a}_\beta)_{,\alpha} - (u^n \boldsymbol{a}_3)_{,\alpha} = \boldsymbol{a}_\alpha - \left( u^\lambda|_\alpha - u^n b_\alpha^\lambda \right)\boldsymbol{a}_\lambda - \left( u^\lambda b_{\lambda\alpha} + u_{,\alpha}^n \right)\boldsymbol{a}_3 \tag{4}$$

where $\mathbf{b} = b_{\lambda\alpha}\boldsymbol{a}^\lambda \otimes \boldsymbol{a}^\alpha$ is the curvature tensor of the interface $A$ after deformation. Thus, the inverse of the interface deformation gradient is expressed as

$$\mathbf{F}_s^{-1} = \mathbf{A}_\alpha \otimes \boldsymbol{a}^\alpha = \mathbf{i} - \mathbf{u}\nabla_s - \boldsymbol{a}_3 \otimes \mathbf{d} \tag{5}$$

where $\mathbf{i}$ is the unit tensor on interface $A$, $\mathbf{u}\nabla_s = \mathbf{u}_s\nabla_s - u^n\mathbf{b}$ is the surface displacement gradient and $\mathbf{d} = \mathbf{u}_s \cdot \mathbf{b} + u^n \nabla_s$ in the current configuration.

By using the polar decompositions of $\mathbf{F}_s$, the right and left Cauchy–Green tensors of the interface can be defined as $\mathbf{C}_s = \mathbf{U}_s^2 = \mathbf{F}_s^{\mathrm{T}} \cdot \mathbf{F}_s$ and $\mathbf{B}_s = \mathbf{V}_s^2 = \mathbf{F}_s \cdot \mathbf{F}_s^{\mathrm{T}}$, where $\mathbf{U}_s$ and $\mathbf{V}_s$ are called the right and left stretch tensors of the interface, respectively.

### 2.2. Strain measures of the interface

Following the discussion of Seth (1964), the two-dimensional strain tensor can be formulated to characterize the stretching deformation of the interface. In the reference configuration, the Lagrangian strain tensor of the interface can be defined as

$$\mathbf{E}_s^{(m)} = \frac{1}{2m}\left( \mathbf{U}_s^{2m} - \mathbf{i}_0 \right), \quad m \neq 0$$
$$\mathbf{E}_s^{(0)} = \ln \mathbf{U}_s, \quad m = 0 \tag{6}$$

where $m$ is a real number. In particular, when $m = 1$, we obtain the Green strain tensor of the interface

$$\mathbf{E}_s^{(1)} = \frac{1}{2}\left(\mathbf{U}_s^2 - \mathbf{i}_0\right) = \frac{1}{2}(\mathbf{C}_s - \mathbf{i}_0) \tag{7}$$

which furnishes the change of the metric tensor of the interface and will be used in the following section.

Following Steigmann and Ogden (1999), the relative curvature $\boldsymbol{\kappa}$ of the interface can be defined by

$$\boldsymbol{\kappa} = -\mathbf{F}_s^T \cdot \mathbf{b} \cdot \mathbf{F}_s \tag{8}$$

which is the pullback of the curvature tensor $\boldsymbol{b}$ from the current configuration to the reference configuration. Considering $\mathbf{b} = -\boldsymbol{a}_{3,\alpha} \otimes \boldsymbol{a}^\alpha$, Eq. (8) can be rewritten as

$$\boldsymbol{\kappa} = \mathbf{F}_s^T \cdot (\boldsymbol{a}_{3,\alpha} \otimes \mathbf{A}^\alpha) = \mathbf{F}_s^T \cdot (\boldsymbol{a}_3 \tilde{\nabla}_{0s}) \tag{9}$$

where $(\cdot)\tilde{\nabla}_{0s} = (\cdot)_{,\alpha} \otimes \mathbf{A}^\alpha$ that has the same meaning as the differential operator "$\nabla$" used by Gurtin et al. (1998). Similarly, the flexural deformation of an interface is usually characterized by the change of its curvature tensor (Green and Zerna, 1960; Langhaar, 1974). Thus, the Lagrangian curvature strain of the interface can be defined as

$$\boldsymbol{\Lambda} = (b_{\alpha\beta} - B_{\alpha\beta})\mathbf{A}^\alpha \otimes \mathbf{A}^\beta = -\boldsymbol{\kappa} - \mathbf{B} \tag{10}$$

Generally speaking, the stretching and the flexural deformations of the interface are coupled with each other, and the shape of the interface is usually unknown after deformation, making the deformation of an interface quite complicated; thus, the Lagrangian strain measures based on the initial reference configuration are preferable and more convenient for describing the deformation and kinematics of the interface.

## 3. The nonlinear constitutive relation of the interface

The constitutive relation of the interface describes the correlations among interfacial energy, interface stress, and interface strain. Pioneering work in this area can be traced back to the famous Shuttleworth–Herring equation (Shuttleworth, 1950; Herring, 1951) and was used as a foundation for advanced theories by many researchers. Gurtin and Murdoch (1975) derived the constitutive relation of the interface within the framework of the Cauchy elasticity theory. Recently, a comprehensive version of the nonlinear constitutive relation of the interface at finite deformation based on the Green elasticity theory was given by Huang and Wang (2006), as well as the related linearized constitutive relation (Huang and Sun, 2007). Steigmann and Ogden (1999) presented a component form of the constitutive relation for the hemitropic planes and spheres based on their curvature-dependent interfacial energies and a simplified linear version was later given by Chhapadia et al. (2011). Dingreville and Qu (2008) developed a new relationship between the interfacial excess energy and interfacial excess stress for planar interfaces, which accounted for the transverse deformation, transverse stress and the Poisson's effect of the real material interface. For simplicity, the transverse deformation and Poisson's effect of the interface is not considered in the present study.

In this section, the nonlinear constitutive relation of the interface is derived based on the curvature-dependent interfacial energy and the features of the interface stress and bending moment are investigated. Let the excess free energy of the interface per unit area of $A$ in the current configuration be denoted by $\gamma$, which depends not only on the position coordinates but also on the strain and curvature of the interface. For simplicity, the dependence of $\gamma$ on coordinates $(\theta^1, \theta^2)$ will be omitted in the following. Then the interfacial energy per unit area of $A_0$ in the reference configuration can be written as $J_2\gamma$, where $J_2 = \det \mathbf{U}_s$ is the ratio between area elements $dA$ and $dA_0$. In the course of deformation, the variation in the interfacial excess free energy on the area element $dA$ is $\delta(\gamma dA) = \delta(J_2\gamma)dA_0$, which is the reversible work needed to elastically stretch and bend this pre-existing surface element.

$$\delta(J_2\gamma)dA_0 = \left(\mathbf{T}_s^{(m)} : \delta\mathbf{E}_s^{(m)} + \mathbf{M}_s : \delta\boldsymbol{\kappa}\right)dA_0, \tag{11}$$

where $\mathbf{T}_s^{(m)}$ is the interface stress conjugating to the interface strain $\mathbf{E}_s^{(m)}$ and $\mathbf{M}_s$ is the interface bending moment conjugating to the relative curvature $\boldsymbol{\kappa}$.

To elucidate the physical meaning of Eq. (11), let us consider a bimetallic strip. If the strip is initially flat (planar), stretching of the strip exerts an interface stress $\mathbf{T}_s^{(m)}$ on the interface, which induce an interface strain $\mathbf{E}_s^{(m)}$, while the interface remains flat. In this case, $\boldsymbol{\kappa} \equiv \mathbf{0}$, thus $\delta(J_2\gamma) = \mathbf{T}_s^{(m)} : \delta\mathbf{E}_s^{(m)}$. However, a pure bending of the strip will obviously exert a bending moment $\mathbf{M}_s$ on the interface, which will induce $\boldsymbol{\kappa}$. The applied bending moment may also exert an interface stress $\mathbf{T}_s^{(m)}$ if the interface microstructure is not symmetric with respect to the interface, indicating a coupling between the stretching and flexural responses of the interface. On the other hand, if the bimetallic strip is initially curved, a stretching of the the strip will exert both $\mathbf{T}_s^{(m)}$ and $\mathbf{M}_s$, which would induce both $\mathbf{E}_s^{(m)}$ and $\boldsymbol{\kappa}$. Therefore, as thermodynamic driving forces, the interface stress and the interface bending moment are independent. Their respective conjugates are the stretching and the flexural deformation. However, we note that interface stress may also cause flexural deformation and vice versa if the interface is curved.

The derivation of the constitutive relation of the interface at finite deformation from Eq. (11) is straightforward in the framework of Green elasticity, which gives

$$\mathbf{T}_s^{(m)} = \frac{\partial(J_2\gamma)}{\partial\mathbf{E}_s^{(m)}}, \quad \mathbf{M}_s = \frac{\partial(J_2\gamma)}{\partial\mathbf{\kappa}} \tag{12}$$

where the Lagrangian description has been used and $J_2\gamma$ represents the interfacial energy per unit area in the reference configuration. In particular, the Piola–Kirchhoff stresses of the first and second kinds are given by

$$\mathbf{S}_s = 2\mathbf{F}_s \cdot \frac{\partial(J_2\gamma)}{\partial\mathbf{C}_s}, \quad \mathbf{T}_s^{(1)} = \frac{\partial(J_2\gamma)}{\partial\mathbf{E}_s^{(1)}} = 2\frac{\partial(J_2\gamma)}{\partial\mathbf{C}_s} \tag{13}$$

In the current configuration, the Cauchy stress of the interface can be expressed as

$$\mathbf{\sigma}_s = \frac{1}{J_2}\mathbf{F}_s \cdot \mathbf{T}_s^{(1)} \cdot \mathbf{F}_s^{\mathrm{T}} = \frac{2}{J_2}\mathbf{F}_s \cdot \frac{\partial(J_2\gamma)}{\partial\mathbf{C}_s} \cdot \mathbf{F}_s^{\mathrm{T}} \tag{14}$$

and the Eulerian bending moment of the interface is defined as

$$\mathbf{m}_s = \frac{1}{J_2}\mathbf{F}_s \cdot \mathbf{M}_s \cdot \mathbf{F}_s^{\mathrm{T}} = \mathbf{F}_s \cdot \frac{\partial\gamma}{\partial\mathbf{\kappa}} \cdot \mathbf{F}_s^{\mathrm{T}} \tag{15}$$

It is noted that the above expressions are valid for anisotropic interfaces as well.

A detailed analysis of the material symmetry of the interface (Steigmann, 2001) indicates that the interfacial energy $J_2\gamma$ is generally not an isotropic scalar-valued tensor function relative to the reference configuration. Since the interfacial energy $J_2\gamma$ is a rather complicated function of $\mathbf{C}_s$ and $\mathbf{\kappa}$, its explicit expression should be determined by the physical properties of the real material interfaces. In order to simplify this problem while still capturing the main physical features of the constitutive relation, it can be assumed that the material interface is hemitropic relative to the reference configuration. Hence, the interfacial energy $J_2\gamma$ can be expressed as a function of the six invariants of the right Cauchy–Green tensor $\mathbf{C}_s$ and relative curvature $\mathbf{\kappa}$ (Zheng, 1993):

$$J_2\gamma(\mathbf{C}_s, \mathbf{\kappa}) = J_2\gamma(I_1, I_2, I_3, I_4, I_5, I_6) \tag{16}$$

The six scalar invariants are defined as

$$I_1 = \mathrm{tr}\mathbf{C}_s, I_2 = \det\mathbf{C}_s, I_3 = \mathrm{tr}\mathbf{\kappa}, I_4 = \det\mathbf{\kappa}, I_5 = \mathrm{tr}(\mathbf{C}_s \cdot \mathbf{\kappa}), I_6 = \mathrm{tr}(\mathbf{C}_s \cdot \mathbf{\kappa} \cdot \mathbf{\varepsilon}). \tag{17}$$

where $\mathbf{\varepsilon}$ denotes the permutation tensor on the surface $A_0$. Noting that

$$\frac{\partial I_1}{\partial\mathbf{C}_s} = \mathbf{i}_0, \frac{\partial I_2}{\partial\mathbf{C}_s} = I_2\mathbf{C}_s^{-1}, \frac{\partial I_3}{\partial\mathbf{\kappa}} = \mathbf{i}_0, \frac{\partial I_4}{\partial\mathbf{\kappa}} = I_4\mathbf{\kappa}^{-1}, \frac{\partial J_2}{\partial\mathbf{C}_s} = \frac{1}{2}J_2\mathbf{C}_s^{-1},$$

$$\frac{\partial I_5}{\partial\mathbf{C}_s} = \mathbf{\kappa}, \frac{\partial I_5}{\partial\mathbf{\kappa}} = \mathbf{C}_s, \frac{\partial I_6}{\partial\mathbf{C}_s} = \mathbf{\varepsilon}^{\mathrm{T}} \cdot \mathbf{\kappa} = -\mathbf{\varepsilon} \cdot \mathbf{\kappa}, \frac{\partial I_6}{\partial\mathbf{\kappa}} = \mathbf{C}_s \cdot \mathbf{\varepsilon}^{\mathrm{T}} = -\mathbf{C}_s \cdot \mathbf{\varepsilon} \tag{18}$$

we obtain

$$\mathbf{T}_s^{(1)} = 2J_2\left[\frac{\partial\gamma}{\partial I_1}\mathbf{i}_0 + \left(I_2\frac{\partial\gamma}{\partial I_2} + \frac{\gamma}{2}\right)\mathbf{C}_s^{-1} + \frac{\partial\gamma}{\partial I_2}\mathbf{\kappa} + \frac{1}{2}\frac{\partial\gamma}{\partial I_6}(\mathbf{\kappa} \cdot \mathbf{\varepsilon} - \mathbf{\varepsilon} \cdot \mathbf{\kappa})\right] \tag{19}$$

$$\mathbf{M}_s = J_2\left[\frac{\partial\gamma}{\partial I_3}\mathbf{i}_0 + I_4\frac{\partial\gamma}{\partial I_4}\mathbf{\kappa}^{-1} + \frac{\partial\gamma}{\partial I_5}\mathbf{C}_s + \frac{1}{2}\frac{\partial\gamma}{\partial I_6}(\mathbf{\varepsilon} \cdot \mathbf{C}_s - \mathbf{C}_s \cdot \mathbf{\varepsilon})\right] \tag{20}$$

where it should be pointed out that only the symmetric parts of the stress and bending moment are retained because their skew-symmetric parts do not contribute to the incremental interfacial energy presented in Eq. (11).

The Cauchy stress and Eulerian bending moment of the interface are

$$\mathbf{\sigma}_s = 2\left[\frac{\partial\gamma}{\partial I_1}\mathbf{B}_s + \left(I_2\frac{\partial\gamma}{\partial I_2} + \frac{\gamma}{2}\right)\mathbf{i} - \frac{\partial\gamma}{\partial I_5}\mathbf{B}_s \cdot \mathbf{b} \cdot \mathbf{B}_s + \frac{1}{2}\frac{\partial\gamma}{\partial I_6}J_2(\mathbf{\mu} \cdot \mathbf{b} \cdot \mathbf{B}_s - \mathbf{B}_s \cdot \mathbf{b} \cdot \mathbf{\mu})\right] \tag{21}$$

$$\mathbf{m}_s = \frac{\partial\gamma}{\partial I_3}\mathbf{B}_s - I_4\frac{\partial\gamma}{\partial I_4}\mathbf{b}^{-1} + \frac{\partial\gamma}{\partial I_5}\mathbf{B}_s^2 + \frac{1}{2}\frac{\partial\gamma}{\partial I_6}J_2(\mathbf{\mu} \cdot \mathbf{B}_s - \mathbf{B}_s \cdot \mathbf{\mu}) \tag{22}$$

where $\mathbf{\mu}$ denotes the permutation tensor on the surface $A$. By using the Cayley–Hamilton theorem, Eq. (20) can be rewritten as

$$\mathbf{M}_s = J_2\left[\left(\frac{\partial\gamma}{\partial I_3} + I_3\frac{\partial\gamma}{\partial I_4}\right)\mathbf{i}_0 - \frac{\partial\gamma}{\partial I_4}\mathbf{\kappa} + \frac{\partial\gamma}{\partial I_5}\mathbf{C}_s + \frac{1}{2}\frac{\partial\gamma}{\partial I_6}(\mathbf{\varepsilon} \cdot \mathbf{C}_s - \mathbf{C}_s \cdot \mathbf{\varepsilon})\right] \tag{23}$$

The constitutive equation above clearly shows that there exists a stretching-bending coupling due to the curvature-dependent nature of the interfacial energy. Even when there is no in-plane stretching deformation, the residual interface stress may still depend on the flexural deformation. Furthermore, there exists an interface bending moment that characterizes the resistance to bending of the interface.

Unlike in the classical theory of elastic surfaces and shells, the constitutive equations above include the residual stress and the residual bending moment in the interface. In the initial state without external load, the current and the reference

configurations coincide, thus giving us $\mathbf{C}_s = \mathbf{i}_0 = \mathbf{i} = \mathbf{B}_s$, $\mathbf{B} = -\boldsymbol{\kappa} = \mathbf{b}$ and $\boldsymbol{\varepsilon} = \boldsymbol{\mu}$. The scalar invariants reduce to

$$J_2 = 1, \quad I_1 = 2, \quad I_2 = 1, \ I_3 = -2H_0, \quad I_4 = K_0, \quad I_5 = -2H_0, \quad I_6 = 0 \tag{24}$$

where $H_0$ and $K_0$ are the mean and the Gaussian curvatures of the interface $A_0$, respectively. Hence, the residual interface stress and the residual interface bending moment can be written as

$$\boldsymbol{\sigma}_s^* = (\gamma_0 + 2\gamma_1 + 2\gamma_2)\mathbf{i}_0 - 2\gamma_5\mathbf{B} + \gamma_6(\boldsymbol{\varepsilon} \cdot \mathbf{B} - \mathbf{B} \cdot \boldsymbol{\varepsilon}) \tag{25}$$

$$\mathbf{m}_s^* = (\gamma_3 + \gamma_5)\mathbf{i}_0 - K_0\gamma_4\mathbf{B}^{-1} = (\gamma_3 + \gamma_5 - 2\gamma_4 H_0)\mathbf{i}_0 + \gamma_4\mathbf{B} \tag{26}$$

where $\gamma_0$ is the initial interfacial excess free energy and $\gamma_i = \partial\gamma/\partial I_i (i=1–6)$ reflect the natures of the solid interfaces. All of these parameters describe the intrinsic properties of the interfaces and are determined by the joining materials, the adhering conditions and the initial curvature of the interface. These two residual terms $\boldsymbol{\sigma}_s^*$ and $\mathbf{m}_s^*$ indicate that the interface has the inclination to stretch and bend even though it cannot exist independently without the joining bulk materials. Unlike the cases in the literature (Gurtin and Murdoch, 1975; Huang and Wang, 2006, 2013), the residual interface stress is not homogeneous at the interface because it is curvature-dependent.

To understand the physical interpretations of the residual interface stress and the residual interface bending moment, it is elucidative to imagine that an infinitesimally thin slice of material containing the interface is cut from the bulk bimaterial. When standing alone, this thin slice would release its residual interface stress by changing its own area. In other words, the residual interface stress is what prevented the interface to relax in its own plane when the interface is surrounded by the bulks materials that form the interface. Furthermore, if the atomic arrangement on and near the interface is not symmetric with respect to the interface plane, the stand-alone thin slice would also change its own curvature due to the microstructural asymmetry with respect to the interface plane, thus completely releases its residual interface bending moment. In other words, the residual interface bending moment is what prevented the interface to relax flexurally when the interface is surrounded by the bulk materials that form the interface.

## 4. The residual elastic field induced by the interfacial energy

Recently, studies (Huang and Wang, 2006, 2013; Huang and Sun, 2007) showed that, in a multi-phase hyperelastic body, that is free from any external load, the excess interfacial free energy and the corresponding residual interface stress are not zero, as indicated in Section 3. Therefore, there exists a self-equilibrium stress field in the bulk body because of the existence of residual interface stress. Thus, the elastic strain energy of the bulk body does not vanish even in the initial state. We will call this elastic field induced by the residual interface stress the "residual" elastic field in the bulk.

As has already been demonstrated by Hoger (1986, 1993), the elastic properties of a residually stressed body are fundamentally different from those of an initially stress-free body. The elastic tensors in the constitutive equations can depend explicitly on the residual stress, which are different from their counterparts in the classical theory. In Hoger's work, notably, no assumption was made about the origin of the residual stress and the interface effect in the heterogeneous body was not considered.

Therefore, the interfacial energy-induced residual elastic field in the body is another critically important characteristic of heterogeneous nano-structured materials. Since residual stresses are presented in heterogeneous materials where the interface effects cannot be neglected, elasticity problems in such materials cannot be treated by simply employing the classical theory of elasticity. Nevertheless, this fact seems to have been neglected by a number of previous researchers who have studied the interface effect in nano-structured materials.

To facilitate the description of the deformation induced by the interfacial energy in a heterogeneous solid, one can hypothetically split the solid into homogenous pieces along its interface, and imagine that they have been returned to their stress-free states. It should be emphasized that in general such a process cannot be realized in practice, since it is assumed that the atomic-level micro-structures of the surfaces, which would be obtained by splitting an interface, would have the same micro-structures as those of their respective interior parts. Thus the above splitting process is only a thought experiment, based on which, we can suggest a "fictitious stress-free configuration", symbolized by $\kappa$. This imaginary "fictitious stress-free configuration" may not exist because splitting a solid would inevitably create new surfaces, and the new surface energy would in turn induce a new residual stress field in the bulk, but this fictitious stress-free configuration provides useful and meaningful way to describe and calculate the residual elastic field induced by interfacial energy.

Let $\mathbf{F}^*$ denotes the deformation gradient from $\kappa_*$ to $\kappa_0$ and $\boldsymbol{F}$ denotes the deformation gradient from $\kappa_0$ to $\kappa$. From the above discussions, it is seen that the elastic stress field in the heterogeneous solid under external loads should depend on the deformation gradient $\mathbf{F} \cdot \mathbf{F}^*$. Hence the potential function of the hyperelastic solid should be expressed as $\psi_0 = \psi_0(\tilde{\mathbf{C}})$, where $\tilde{\mathbf{C}} = (\mathbf{F} \cdot \mathbf{F}^*)^{\mathrm{T}} \cdot (\mathbf{F} \cdot \mathbf{F}^*)$ denotes the right Cauchy–Green tensor relative to $\kappa_*$. Therefore, the first Piola–Kirchhoff stress relative to the reference configuration $\kappa_0$ is

$$\mathbf{S}^0 = 2\rho_0 \mathbf{F} \cdot \mathbf{F}^* \cdot \frac{\partial\psi_0}{\partial\tilde{\mathbf{C}}} \cdot \mathbf{F}^{*\mathrm{T}} \tag{27}$$

and the Cauchy stress corresponding to the current configuration $\kappa$ is

$$\boldsymbol{\sigma} = 2\rho \mathbf{F} \cdot \mathbf{F}^* \cdot \frac{\partial \psi_0}{\partial \tilde{\mathbf{C}}} \cdot \mathbf{F}^{*T} \cdot \mathbf{F}^{T} \tag{28}$$

In the above expressions, $\rho_0$ and $\rho$ denote the mass densities of the bulk solid in the configurations $\kappa_0$ and $\kappa$, respectively. Conservation of mass yields $\rho_0/\rho = \det \mathbf{F}$.

The residual elastic stress field is the solution corresponding to the unloaded state when the current configuration coincides with the reference configuration. Setting $\mathbf{F} = \mathbf{I}$ in Eq. (28), the residual stress $\boldsymbol{\sigma}^*$ can be expressed as

$$\boldsymbol{\sigma}^* = 2\rho_0 \mathbf{F}^* \cdot \left( \left. \frac{\partial \psi_0}{\partial \tilde{\mathbf{C}}} \right|_{\mathbf{F} = \mathbf{I}} \right) \cdot \mathbf{F}^{*T} \tag{29}$$

where $\boldsymbol{I}$ is the second-order identity tensor in the three dimensional Euclidean space.

## 5. The equilibrium equation for the interface

Besides the constitutive relation of the interface, the second fundamental equation of the interface is the equilibrium equation, which is usually called the generalized Young–Laplace equation. The generalized Young–Laplace equation describes the equilibrium relationship between the interface stress and the stress in the bulk. In fact, the mathematical structure of this equation is very similar to that of the equilibrium equation of an elastic thin shell but they have different physical meanings and application backgrounds. The generalized Young–Laplace equation reflects the effect of interface stress on the heterogeneous materials and is mainly applied to nanostructures. In the classical interface stress theory, this equation is of crucial importance because many size-dependent properties of nano-structured materials are well explained by it.

In this section, the generalized Young–Laplace equation will be derived by the principle of minimum potential energy, which requires a new energy functional that accounts for the interfacial energy effect in heterogeneous hyperelastic solids. This energy functional consists of three parts: first, the interfacial energy, which depends not only on the interface strain but also on the interface curvature; second, the elastic strain energy of the body, which includes the residual elastic field induced by the interfacial energy; and third, the potential of the external loads. Therefore, this energy functional for can be written as

$$\Pi(\mathbf{u}) = \int_{A_0} J_2 \gamma(\mathbf{C}_s, \boldsymbol{\kappa}) \mathrm{d}A_0 + \int_{v_0} \rho_0 \psi_0(\tilde{\mathbf{C}}) \mathrm{d}v_0 - \int_{v_0} \rho_0 \mathbf{f} \cdot \mathbf{u} \mathrm{d}v_0 - \int_{\partial v_{0T}} {}_0\bar{\mathbf{t}} \cdot \mathbf{u} \mathrm{d}s_0 \tag{30}$$

where $\boldsymbol{u}$ is the displacement, $\mathbf{f}$ is the body force per unit mass and ${}_0\bar{\mathbf{t}}$ is the traction on the boundary. It should be noted that the displacement $\boldsymbol{u}$ is calculated for the reference configuration to the current configuration. As indicated before, even in the initial state when there is no displacement or external load, the energy functional does not vanish.

Accordingly, we have the following proposition: for any admissible displacement field $\boldsymbol{u}$ that satisfies the prescribed $\bar{\mathbf{u}}_0$ on the boundary $\partial v_{0u}$, the energy functional takes a stationary value when $\boldsymbol{u}$ is that of the equilibrium state of the system, which is subjected to a body force $\mathbf{f}$ in $v_0$ and a traction ${}_0\bar{\mathbf{t}}$ on its boundary $\partial v_{0T}$.

### 5.1. The Lagrangian description of the interface equilibrium equation

Let the displacement $\boldsymbol{u}$ be subjected to a variation $\delta \boldsymbol{u}_0$. This variation can be decomposed into a sum of $\delta \boldsymbol{u}_{0s}$ in the tangential direction and $\delta u_0^n \mathbf{A}_3$ along the normal direction in the reference configuration. Then, in the Lagrangian description, the variation of the energy functional in Eq. (30) is

$$\delta \Pi(\mathbf{u}) = \int_{A_0} \delta(J_2 \gamma) \mathrm{d}A_0 + \int_{v_0} \delta(\rho_0 \psi_0) \mathrm{d}v_0 - \int_{v_0} \delta \mathbf{u} \cdot (\rho_0 \mathbf{f}) \mathrm{d}v_0 - \int_{\partial v_{0T}} (\delta \mathbf{u} \cdot {}_0\bar{\mathbf{t}}) \mathrm{d}s_0 \tag{31}$$

The integrand of the first term on the right side of Eq. (31) can be written as

$$\delta(J_2 \gamma) = \frac{\partial(J_2 \gamma)}{\partial \mathbf{C}_s} : \delta \mathbf{C}_s + \frac{\partial(J_2 \gamma)}{\partial \boldsymbol{\kappa}} : \delta \boldsymbol{\kappa} = \frac{1}{2} \mathbf{T}_s^{(1)} : \delta \mathbf{C}_s + \mathbf{M}_s : \delta \boldsymbol{\kappa} \tag{32}$$

In detail, the first variation term on the right side of Eq. (32) can be rewritten as

$$\frac{\partial(J_2 \gamma)}{\partial \mathbf{C}_s} : \delta \mathbf{C}_s = \frac{1}{2} \mathbf{T}_s^{(1)} : \delta \mathbf{C}_s = \left( \mathbf{F}_s \cdot \mathbf{T}_s^{(1)} \right) : \delta \mathbf{F}_s = \mathbf{S}_s : \delta \mathbf{F}_s \tag{33}$$

Since $\boldsymbol{F}_s$ is expressed as a sum of the in-plane term $\mathbf{F}_s^{(in)}$ and out-plane term $\mathbf{F}_s^{(ou)}$, the first Piola–Kirchhoff interface stress $\boldsymbol{S}_s$ is also a "two-point" tensor, and can be decomposed into an in-plane term $\mathbf{S}_s^{(in)} = \mathbf{F}_s^{(in)} \cdot \mathbf{T}_s^{(1)}$ and an out-plane term $\mathbf{S}_s^{(ou)} = \mathbf{F}_s^{(ou)} \cdot \mathbf{T}_s^{(1)}$. Therefore, in view of Eqs. (2) and (3), (33) can be further given by

$$\begin{aligned} \mathbf{S}_s : \delta \mathbf{F}_s &= \mathbf{S}_s^{(in)} : \delta \mathbf{F}_s^{(in)} + \mathbf{S}_s^{(ou)} : \delta \mathbf{F}_s^{(ou)} \\ &= \left( \delta \mathbf{u}_{0s} \cdot \mathbf{S}_s^{(in)} \right) \cdot \nabla_{0s} + \left( \delta u_0^n \mathbf{A}_3 \cdot \mathbf{S}_s^{(ou)} \right) \cdot \nabla_{0s} - \delta \mathbf{u}_{0s} \cdot \left( \mathbf{S}_s^{(in)} \cdot \nabla_{0s} - \mathbf{A}_3 \cdot \mathbf{S}_s^{(ou)} \cdot \mathbf{B} \right) - \delta u_0^n \left( \mathbf{S}_s^{(in)} : \mathbf{B} + \left( \mathbf{A}_3 \cdot \mathbf{S}_s^{(ou)} \right) \cdot \nabla_{0s} \right). \end{aligned} \tag{34}$$

Now consider a region $\Omega_0$ enclosed by an arbitrary closed smooth curve $\partial\Omega_0$ on the interface $A_0$ in the reference configuration. By using the Green–Stokes theorem, we have

$$
\int_{A_0} (\mathbf{S}_s : \delta\mathbf{F}_s)\mathrm{d}A_0 = \int_{A_0} \delta\mathbf{u}_{0s} \cdot \left[ -\mathbf{S}_s^{(in)} \cdot \nabla_{0s} + \mathbf{B} \cdot \left(\mathbf{A}_3 \cdot \mathbf{S}_s^{(ou)}\right) \right] \mathrm{d}A_0
$$
$$
+ \int_{A_0} \delta u_0^n \left[ -\mathbf{S}_s^{(in)} : \mathbf{B} - \left(\mathbf{A}_3 \cdot \mathbf{S}_s^{(ou)}\right) \cdot \nabla_{0s} \right] \mathrm{d}A_0
$$
$$
- \int_{\partial\Omega_0} \delta\mathbf{u}_{0s} \cdot [\![ \mathbf{S}_s^{(in)} ]\!] \cdot \mathbf{n}_0 \mathrm{d}l_0 - \int_{\partial\Omega_0} \delta u_0^n [\![ \mathbf{A}_3 \cdot \mathbf{S}_s^{(ou)} ]\!] \cdot \mathbf{n}_0 \mathrm{d}l_0 \tag{35}
$$

where $\mathrm{d}l_0$ is the differential element of the arc length on $\partial\Omega_0$, $\mathbf{n}_0 = \mathbf{l}_0 \times \mathbf{A}_3$ is the unit normal vector of the curve $\partial\Omega_0$ with $\mathbf{l}_0$ being the unit tangent vector of $\partial\Omega_0$ and $[\![ \cdot ]\!]$ represents the discontinuities across the curve $\partial\Omega_0$. Since the interface stress is continuous across the closed curve $\partial\Omega_0$, the boundary integrals vanish in Eq. (35).

Next, the second variation term on the right side of Eq. (32) can be rewritten as

$$
\frac{\partial(J_2\gamma)}{\partial\boldsymbol{\kappa}} : \delta\boldsymbol{\kappa} = \mathbf{M}_s : \delta\boldsymbol{\kappa} = (\boldsymbol{a}_3 \tilde{\nabla}_{0s}) \cdot \mathbf{M}_s : \delta\mathbf{F}_s + \mathbf{F}_s \cdot \mathbf{M}_s : (\delta\boldsymbol{a}_3 \tilde{\nabla}_{0s}) \tag{36}
$$

in which the Eq. (9) is used. By employing the Lagrangian description of normal vector $\boldsymbol{a}_3$ shown in Eq. (A.2) (see in Appendix A), we have

$$
\boldsymbol{a}_3 \tilde{\nabla}_{0s} = \left[ -\left(\frac{\mathbf{Z}}{J_2}\right)\nabla_{0s} - \left(\frac{X}{J_2}\right)\mathbf{B} \right] + \mathbf{A}_3 \otimes \left[ \left(\frac{X}{J_2}\right)\nabla_{0s} - \frac{1}{J_2}\mathbf{B} \cdot \mathbf{Z} \right] \tag{37}
$$

where $\mathbf{Z} = \boldsymbol{\varepsilon}^{\mathrm{T}} \cdot \mathbf{F}_s^{(in)} \cdot \boldsymbol{\varepsilon} \cdot \mathbf{D}$ and $X = \det\mathbf{F}_s^{(in)}$. The in-plane and out-plane terms of $\boldsymbol{a}_3 \tilde{\nabla}_{0s}$ are

$$
-\left(\frac{\mathbf{Z}}{J_2}\right)\nabla_{0s} - \left(\frac{X}{J_2}\right)\mathbf{B} = \boldsymbol{a}_3\nabla_{0s}, \quad \mathbf{A}_3 \otimes \left[ \left(\frac{X}{J_2}\right)\nabla_{0s} - \frac{1}{J_2}\mathbf{B} \cdot \mathbf{Z} \right] = \boldsymbol{a}_3 \tilde{\nabla}_{0s} - \boldsymbol{a}_3\nabla_{0s} \tag{38}
$$

Then the first term on the right side of Eq. (36) can be expressed as

$$
(\boldsymbol{a}_3 \tilde{\nabla}_{0s}) \cdot \mathbf{M}_s : \delta\mathbf{F}_s = \mathbf{N}_s^{(in)} : \delta\mathbf{F}_s^{(in)} + \mathbf{N}_s^{(ou)} : \delta\mathbf{F}_s^{(ou)} \tag{39}
$$

where $\mathbf{N}_s^{(in)} = (\boldsymbol{a}_3\nabla_{0s}) \cdot \mathbf{M}_s$ and $\mathbf{N}_s^{(ou)} = (\boldsymbol{a}_3 \tilde{\nabla}_{0s} - \boldsymbol{a}_3\nabla_{0s}) \cdot \mathbf{M}_s$, and the second term on the right side of Eq. (36) can be expressed as

$$
\mathbf{F}_s \cdot \mathbf{M}_s : (\delta\boldsymbol{a}_3 \tilde{\nabla}_{0s}) = \mathbf{M}_s^{(in)} : \left[ -\delta\left(\frac{\mathbf{Z}}{J_2}\right)\nabla_{0s} - \delta\left(\frac{X}{J_2}\right)\mathbf{B} \right] + \mathbf{M}_s^{(ou)} : \mathbf{A}_3 \otimes \left[ \delta\left(\frac{X}{J_2}\right)\nabla_{0s} - \mathbf{B} \cdot \delta\left(\frac{\mathbf{Z}}{J_2}\right) \right] \tag{40}
$$

where $\mathbf{M}_s^{(in)} = \mathbf{F}_s^{(in)} \cdot \mathbf{M}_s$ and $\mathbf{M}_s^{(ou)} = \mathbf{F}_s^{(ou)} \cdot \mathbf{M}_s$.

After some mathematical manipulations, Eq. (40) can be rewritten as

$$
\mathbf{F}_s \cdot \mathbf{M}_s : (\delta\boldsymbol{a}_3 \tilde{\nabla}_{0s}) = \delta\left(\frac{\mathbf{Z}}{J_2}\right) \cdot \left(\mathbf{M}_s^{(in)} \cdot \nabla_{0s} - \mathbf{A}_3 \cdot \mathbf{M}_s^{(ou)} \cdot \mathbf{B}\right) - \delta\left(\frac{X}{J_2}\right)\left[ \mathbf{M}_s^{(in)} : \mathbf{B} + \left(\mathbf{A}_3 \cdot \mathbf{M}_s^{(ou)}\right) \cdot \nabla_{0s} \right]
$$
$$
+ \left[ -\delta\left(\frac{\mathbf{Z}}{J_2}\right) \cdot \mathbf{M}_s^{(in)} + \delta\left(\frac{X}{J_2}\right)\mathbf{A}_3 \cdot \mathbf{M}_s^{(ou)} \right] \cdot \nabla_{0s} \tag{41}
$$

For simplicity, we denote that

$$
\mathbf{T}_1 = \mathbf{M}_s^{(in)} \cdot \nabla_{0s} - \mathbf{A}_3 \cdot \mathbf{M}_s^{(ou)} \cdot \mathbf{B}, T_2 = \mathbf{M}_s^{(in)} : \mathbf{B} + \left(\mathbf{A}_3 \cdot \mathbf{M}_s^{(ou)}\right) \cdot \nabla_{0s} \tag{42}
$$

Thereby the first two terms on the right side of Eq. (41) can be rewritten as

$$
\delta\left(\frac{\mathbf{Z}}{J_2}\right) \cdot \mathbf{T}_1 - \delta\left(\frac{X}{J_2}\right)T_2 = \delta\mathbf{Z} \cdot \left(\frac{\mathbf{T}_1}{J_2}\right) + \delta J_2 \left(\frac{-\mathbf{Z} \cdot \mathbf{T}_1 + XT_2}{J_2^2}\right) - \delta X\left(\frac{T_2}{J_2}\right) \tag{43}
$$

By using the related variation formulas given in Appendix B, the first term on the right of Eq. (43) reduces to

$$
\delta\mathbf{Z} \cdot \left(\frac{\mathbf{T}_1}{J_2}\right) = \mathbf{P}_s^{(in)} : \delta\mathbf{F}_s^{(in)} + \mathbf{P}_s^{(ou)} : \delta\mathbf{F}_s^{(ou)} \tag{44}
$$

where

$$
\mathbf{P}_s^{(in)} = \frac{1}{J_2}\left[ \mathrm{tr}(\mathbf{T}_1 \otimes \mathbf{D})\mathbf{i}_0 - (\mathbf{T}_1 \otimes \mathbf{D})^{\mathrm{T}} \right], \mathbf{P}_s^{(ou)} = \frac{1}{J_2}(\mathbf{A}_3 \otimes \mathbf{T}_1) \cdot \left[ \mathrm{tr}(\mathbf{F}_s^{(in)})\mathbf{i}_0 - (\mathbf{F}_s^{(in)})^{\mathrm{T}} \right] \tag{45}
$$

and the second term on the right side of Eq. (43) reduces to

$$
\delta J_2 \left(\frac{-\mathbf{Z} \cdot \mathbf{T}_1 + XT_2}{J_2^2}\right) = \mathbf{F}_s \cdot \mathbf{L}_s : \delta\mathbf{F}_s = \mathbf{L}_s^{(in)} : \delta\mathbf{F}_s^{(in)} + \mathbf{L}_s^{(ou)} : \delta\mathbf{F}_s^{(ou)} \tag{46}
$$

where

$$
\mathbf{L}_s = \frac{1}{J_2^3}(-\mathbf{Z} \cdot \mathbf{T}_1 + XT_2)(I_1\mathbf{i}_0 - \mathbf{C}_s), \mathbf{L}_s^{(in)} = \mathbf{F}_s^{(in)} \cdot \mathbf{L}_s, \mathbf{L}_s^{(ou)} = \mathbf{F}_s^{(ou)} \cdot \mathbf{L}_s \tag{47}
$$

while the third term on the right side of Eq. (43) reduces to

$$-\delta X\left(\frac{T_2}{J_2}\right) = \frac{1}{2}\mathbf{Q}_s : \delta\mathbf{C}_s^{(in)} = \mathbf{Q}_s^{(in)} : \delta\mathbf{F}_s^{(in)} \tag{48}$$

where

$$\mathbf{Q}_s^{(in)} = -\frac{T_2}{J_2}\left[\mathrm{tr}(\mathbf{F}_s^{(in)})\mathbf{i}_0 - (\mathbf{F}_s^{(in)})^{\mathrm{T}}\right] \tag{49}$$

Substitute Eqs. (44), (46) and (48) into Eq. (43) while considering Eq. (41), and we get

$$\mathbf{F}_s \cdot \mathbf{M}_s : (\delta\boldsymbol{a}_3\tilde{\nabla}_{0s}) = \left(\mathbf{P}_s^{(in)} + \mathbf{L}_s^{(in)} + \mathbf{Q}_s^{(in)}\right) : \delta\mathbf{F}_s^{(in)} + \left(\mathbf{P}_s^{(ou)} + \mathbf{L}_s^{(ou)}\right) : \delta\mathbf{F}_s^{(ou)}$$
$$+ \left[-\delta\left(\frac{\mathbf{Z}}{J_2}\right)\cdot\mathbf{M}_s^{(in)} + \delta\left(\frac{X}{J_2}\right)\mathbf{A}_3\cdot\mathbf{M}_s^{(ou)}\right]\cdot\nabla_{0s} \tag{50}$$

after which we substitute Eqs. (39) and (50) into Eq. (36), and finally obtain

$$\mathbf{M}_s : \delta\boldsymbol{\kappa} = \left(\mathbf{N}_s^{(in)} + \mathbf{P}_s^{(in)} + \mathbf{L}_s^{(in)} + \mathbf{Q}_s^{(in)}\right) : \delta\mathbf{F}_s^{(in)} + \left(\mathbf{N}_s^{(ou)} + \mathbf{P}_s^{(ou)} + \mathbf{L}_s^{(ou)}\right) : \delta\mathbf{F}_s^{(ou)}$$
$$+ \left[-\delta\left(\frac{\mathbf{Z}}{J_2}\right)\cdot\mathbf{M}_s^{(in)} + \delta\left(\frac{X}{J_2}\right)\mathbf{A}_3\cdot\mathbf{M}_s^{(ou)}\right]\cdot\nabla_{0s} \tag{51}$$

For simplicity, we denote that

$$\mathbf{S}_m^{(in)} = \mathbf{N}_s^{(in)} + \mathbf{P}_s^{(in)} + \mathbf{L}_s^{(in)} + \mathbf{Q}_s^{(in)}, \mathbf{S}_m^{(ou)} = \mathbf{N}_s^{(ou)} + \mathbf{P}_s^{(ou)} + \mathbf{L}_s^{(ou)} \tag{52}$$

Thus, Eq. (51) can be rewritten as

$$\mathbf{M}_s : \delta\boldsymbol{\kappa} = \left(\delta\mathbf{u}_{0s}\cdot\mathbf{S}_m^{(in)}\right)\cdot\nabla_{0s} + \left(\delta u_0^n\mathbf{A}_3\cdot\mathbf{S}_m^{(ou)})\right)\cdot\nabla_{0s} - \delta\mathbf{u}_{0s}\cdot\left(\mathbf{S}_m^{(in)}\cdot\nabla_{0s} - \mathbf{A}_3\cdot\mathbf{S}_m^{(ou)}\cdot\mathbf{B}\right)$$
$$- \delta u_0^n(\mathbf{S}_m^{(in)}) : \mathbf{B} + (\mathbf{A}_3\cdot\mathbf{S}_m^{(ou)})\cdot\nabla_{0s}) + \left[-\delta\left(\frac{\mathbf{Z}}{J_2}\right)\cdot\mathbf{M}_s^{(in)} + \delta\left(\frac{X}{J_2}\right)\mathbf{A}_3\cdot\mathbf{M}_s^{(ou)}\right]\cdot\nabla_{0s} \tag{53}$$

while its surface integral is

$$\int_{A_0}(\mathbf{M}_s : \delta\boldsymbol{\kappa})\mathrm{d}A_0 = \int_{A_0}\delta\mathbf{u}_{0s}\cdot\left[-\mathbf{S}_m^{(in)}\cdot\nabla_{0s} + \mathbf{B}\cdot\left(\mathbf{A}_3\cdot\mathbf{S}_m^{(ou)}\right)\right]\mathrm{d}A_0 + \int_{A_0}\delta u_0^n\left[-\mathbf{S}_m^{(in)} : \mathbf{B} - \left(\mathbf{A}_3\cdot\mathbf{S}_m^{(ou)}\right)\cdot\nabla_{0s}\right]\mathrm{d}A_0$$
$$- \int_{\partial\Omega_0}\delta\mathbf{u}_{0s}\cdot\ [\![\mathbf{S}_m^{(in)}]\!]\ \cdot\mathbf{n}_0\mathrm{d}l_0 - \int_{\partial\Omega_0}\delta u_0^n\ [\![\mathbf{A}_3\cdot\mathbf{S}_m^{(ou)}]\!]\ \cdot\mathbf{n}_0\mathrm{d}l_0$$
$$+ \int_{\partial\Omega_0}\left[-\delta\left(\frac{\mathbf{Z}}{J_2}\right)\cdot\ [\![\mathbf{M}_s^{(in)}]\!]\ + \delta\left(\frac{X}{J_2}\right)\ [\![\mathbf{A}_3\cdot\mathbf{M}_s^{(ou)}]\!]\ \right]\cdot\mathbf{n}_0\mathrm{d}l_0 \tag{54}$$

It is noted that the last three boundary integrals on the right side of Eq. (54) vanish because the interface bending moment is also continuous across the closed curve $\partial\Omega_0$.

Finally, we derive the variation of the second term on the right side of Eq. (31). Noting that

$$\delta(\rho_0\psi_0) = \mathbf{S}^0 : (\delta\mathbf{u}\nabla_0) = (\mathrm{det}\mathbf{F})\boldsymbol{\sigma} : (\delta\mathbf{u}\nabla) \tag{55}$$

and by the conservation of mass, we have

$$\int_{v_0}\delta(\rho_0\psi_0)\mathrm{d}v_0 = \int_{\partial v_{0T}}\delta\mathbf{u}\cdot(\mathbf{S}^0\cdot{}_0\mathbf{N})\mathrm{d}S_0 - \int_{A_0}\delta\mathbf{u}\cdot\ [\![\mathbf{S}^0]\!]\ \cdot\mathbf{A}_3\mathrm{d}A_0 - \int_{v_0}\delta\mathbf{u}\cdot(\mathbf{S}^0\cdot\nabla_0)\mathrm{d}v_0 \tag{56}$$

where $\nabla_0$ is the gradient operator in three-dimensional Euclidean space and $_0\boldsymbol{N}$ is the unit normal vector to the boundary in the reference configuration. $[\![\mathbf{S}^0]\!]$ represents the discontinuity of the first Piola–Kirchhoff stress across the interface $A_0$.

Substitute Eqs. (35), (54) and (56) into the Eq. (31), and consider the arbitrariness of $\delta\boldsymbol{u}_0$, it is seen that the vanishing of the variation of the energy functional is equivalent to the following equations:

(i) The equilibrium equation of the body and the mechanical boundary condition

$$\mathbf{S}^0\cdot\nabla_0 + \rho_0\,\mathbf{f} = 0 \quad (\text{in } v_0)$$
$$\mathbf{S}^0\cdot{}_0\mathbf{N} = {}_0\bar{\mathbf{t}} \quad (\text{on } \partial v_{0T}) \tag{57}$$

(ii) The equilibrium equations of the interface

$$\mathbf{A}_3\cdot\ [\![\mathbf{S}^0]\!]\ \cdot\mathbf{A}_3 = -\left(\mathbf{S}_s^{(in)} + \mathbf{S}_m^{(in)}\right) : \mathbf{B} - \left[\mathbf{A}_3\cdot\left(\mathbf{S}_s^{(ou)} + \mathbf{S}_m^{(ou)}\right)\right]\cdot\nabla_{0s} \quad (\text{on } A_0)$$
$$\mathbf{P}_0\cdot\ [\![\mathbf{S}^0]\!]\ \cdot\mathbf{A}_3 = -\left(\mathbf{S}_s^{(in)} + \mathbf{S}_m^{(in)}\right)\cdot\nabla_{0s} + \mathbf{B}\cdot\left[\mathbf{A}_3\cdot\left(\mathbf{S}_s^{(ou)} + \mathbf{S}_m^{(ou)}\right)\right] \quad (\text{on } A_0) \tag{58}$$

where $\mathbf{P}_0 = \mathbf{I} - \mathbf{A}_3 \otimes \mathbf{A}_3$ is the projection operator introduced by Gurtin et al. (1998). It should be mentioned that Eq. (58) can be written in a more compact form

$$\llbracket \mathbf{S}^0 \rrbracket \cdot \mathbf{A}_3 = -(\mathbf{S}_s + \mathbf{S}_m) \cdot \tilde{\nabla}_{0s} \tag{59}$$

where $\mathbf{S}_s = \mathbf{S}_s^{(in)} + \mathbf{S}_s^{(ou)}$ is the first Piola–Kirchhoff interface stress and $\mathbf{S}_m = \mathbf{S}_m^{(in)} + \mathbf{S}_m^{(ou)}$ is the associated interface bending moment. If the curvature-dependence of the interfacial energy is neglected, $\mathbf{S}_m$ vanishes and Eq. (59) reduces to the original form (6.9) in Gurtin and Murdoch (1975). We note that the original equation by Gurtin and Murdoch (1975) is rather abstract in its mathematical form that makes it difficult to interpret and implement in practical applications. In contrast, our Eq. (58) explicitly shows the in-plane and out-plane terms of the interface stress/bending moment and their roles, and curvature-dependence of the equilibrium of the interface. Thus, it has a clearer form that can offer new insight into its physical meanings and enables more convenient applications.

## 5.2. The Eulerian description of the interface equilibrium equation

Discussion of the Eulerian description can also be given similarly as follows. First, the variation of the interface deformation gradient can be written in the form

$$\delta \mathbf{F}_s = \delta \boldsymbol{a}_\alpha \otimes \mathbf{A}^\alpha = (\delta \boldsymbol{a}_\alpha \otimes \boldsymbol{a}^\alpha) \cdot \mathbf{F}_s \tag{60}$$

and the variation of the displacement $\delta \mathbf{u}$ can also be decomposed into a sum of its tangential and normal components in the current configuration:

$$\delta \mathbf{u} = \delta \mathbf{u}_s + \delta \mathbf{u}_n = \delta u^\alpha \boldsymbol{a}_\alpha + \delta u^n \boldsymbol{a}_3 \tag{61}$$

By using the Weingarten formula, we have

$$\delta \boldsymbol{a}_\alpha = (\delta \mathbf{u})_{,\alpha} = \left( \delta u^\beta |_\alpha - \delta u^n b_\alpha^\beta \right) \boldsymbol{a}_\beta + \left( \delta u^\beta b_{\alpha\beta} + \delta u_{,\alpha}^n \right) \boldsymbol{a}_3 \tag{62}$$

Therefore, we obtain

$$(\delta \boldsymbol{a}_\alpha \otimes \boldsymbol{a}^\alpha) = (\delta \mathbf{u} \nabla_s) + \delta d_\alpha \boldsymbol{a}_3 \otimes \boldsymbol{a}^\alpha \tag{63}$$

where $\delta \mathbf{u} \nabla_s = \delta u^\beta |_\alpha \boldsymbol{a}_\beta \otimes \boldsymbol{a}^\alpha - \delta u^n \mathbf{b}$ and $\delta d_\alpha = \delta u^\lambda b_{\lambda\alpha} + \delta u_{,\alpha}^n$.

Since the variation of the first term on the right-hand side of Eq. (31) can be expressed as

$$\int_{A_0} \delta(J_2 \gamma) \mathrm{d}A_0 = \int_{A_0} (\mathbf{S}_s : \delta \mathbf{F}_s) \mathrm{d}A_0 + \int_{A_0} (\mathbf{M}_s : \delta \boldsymbol{\kappa}) \mathrm{d}A_0 \tag{64}$$

The first term on the right side of Eq. (64) can be converted into an Eulerian description

$$\int_{A_0} (\mathbf{S}_s : \delta \mathbf{F}_s) \mathrm{d}A_0 = \int_{A_0} \mathbf{S}_s : [(\delta \boldsymbol{a}_\alpha \otimes \boldsymbol{a}^\alpha) \cdot \mathbf{F}_s] \mathrm{d}A_0$$

$$= \int_A \frac{1}{J_2} \left( \mathbf{S}_s \cdot \mathbf{F}_s^T \right) : (\delta \boldsymbol{a}_\alpha \otimes \boldsymbol{a}^\alpha) \mathrm{d}A = \int_A \boldsymbol{\sigma}_s : (\delta \mathbf{u} \nabla_s) \mathrm{d}A \tag{65}$$

while the second term on the right side of Eq. (64) can also be rewritten as

$$\int_{A_0} (\mathbf{M}_s : \delta \boldsymbol{\kappa}) \mathrm{d}A_0 = -\int_A \left( J_2 m_s^{\alpha\beta} \delta b_{\alpha\beta} \right) \mathrm{d}A = -\int_A \mathbf{m}_s : (\delta b_{\alpha\beta} \boldsymbol{a}^\alpha \otimes \boldsymbol{a}^\beta) \mathrm{d}A \tag{66}$$

Eq. (66) should be further developed. After some tedious calculations, we arrive at $\delta b_{\alpha\beta} = \boldsymbol{a}_3 \cdot (\delta \boldsymbol{a}_\alpha)|_\beta$. Therefore,

$$-\mathbf{m}_s : (\delta b_{\alpha\beta} \boldsymbol{a}^\alpha \otimes \boldsymbol{a}^\beta) = -m_s^{\alpha\beta} \boldsymbol{a}_3 \cdot (\delta \boldsymbol{a}_\alpha)|_\beta = (m_s^{\alpha\beta} \boldsymbol{a}_3)|_\beta \cdot \delta \boldsymbol{a}_\alpha - (m_s^{\alpha\beta} \boldsymbol{a}_3 \cdot \delta \boldsymbol{a}_\alpha)|_\beta \tag{67}$$

where $\left( m_s^{\alpha\beta} \boldsymbol{a}_3 \right)|_\beta \cdot \delta \boldsymbol{a}_\alpha = m_s^{\alpha\beta}|_\beta \boldsymbol{a}_3 \cdot \delta \boldsymbol{a}_\alpha + m_s^{\alpha\beta} (\boldsymbol{a}_3|_\beta) \cdot \delta \boldsymbol{a}_\alpha$. By considering the following two geometrical relations

$$\boldsymbol{a}_3 \cdot \delta \boldsymbol{a}_\alpha = b_\alpha^\beta \delta u_\beta + \delta u_{,\alpha}^n = \delta d_\alpha, \quad (\boldsymbol{a}_3|_\beta) \cdot \delta \boldsymbol{a}_\alpha = -b_\beta^\gamma (\delta u_\gamma |_\alpha - b_{\gamma\alpha} \delta u^n) \tag{68}$$

it is seen that the first term on the right side of Eq. (67) is equivalent to

$$(m_s^{\alpha\beta} \boldsymbol{a}_3)|_\beta \cdot \delta \boldsymbol{a}_\alpha = m_s^{\alpha\beta}|_\beta \delta d_\alpha - m_s^{\alpha\beta} b_\beta^\gamma (\delta u_\gamma |_\alpha - b_{\gamma\alpha} \delta u^n) = \delta \mathbf{d} \cdot (\mathbf{m}_s \cdot \nabla_s) - \mathbf{b} \cdot \mathbf{m}_s : (\delta \mathbf{u} \nabla_s) \tag{69}$$

where $\delta \mathbf{d} = \delta d_\alpha \otimes \boldsymbol{a}^\alpha$, while the second term on the right side of Eq. (67) is equivalent to

$$-(m_s^{\alpha\beta} \boldsymbol{a}_3 \cdot \delta \boldsymbol{a}_\alpha)|_\beta = -(m_s^{\alpha\beta} \delta d_\alpha)|_\beta = -(\delta \mathbf{d} \cdot \mathbf{m}_s) \cdot \nabla_s \tag{70}$$

Consequently,

$$\int_{A_0} (\mathbf{M}_s : \delta \boldsymbol{\kappa}) \mathrm{d}A_0 = \int_A \left[ \delta \mathbf{d} \cdot (\mathbf{m}_s \cdot \nabla_s) - \mathbf{b} \cdot \mathbf{m}_s : (\delta \mathbf{u} \nabla_s) - (\delta \mathbf{d} \cdot \mathbf{m}_s) \cdot \nabla_s \right] \mathrm{d}A \tag{71}$$

Now consider a region $\Omega$ enclosed by a closed smooth curve $\partial\Omega$ on the interface $A$. From the Green–Stokes theorem, we learn that Eqs. (65) and (71) can be further rewritten as

$$\int_{A_0}(\mathbf{S}_s : \delta\mathbf{F}_s)\mathrm{d}A_0 = -\int_{\partial\Omega}\delta\mathbf{u}_s\cdot[\![\boldsymbol{\sigma}_s]\!]\cdot\mathbf{n}\mathrm{d}l - \int_A[\delta\mathbf{u}_s\cdot(\boldsymbol{\sigma}_s\cdot\nabla_s) + \delta u^n(\boldsymbol{\sigma}_s : \mathbf{b})]\mathrm{d}A \tag{72}$$

$$\int_{A_0}(\mathbf{M}_s : \delta\boldsymbol{\kappa})\mathrm{d}A_0 = \int_A\delta\mathbf{u}_s\cdot[(\mathbf{b}\cdot\mathbf{m}_s)\cdot\nabla_s - \mathbf{b}\cdot(\mathbf{m}_s\cdot\nabla_s)]\mathrm{d}A + \int_A\delta u^n[(\mathbf{b}\cdot\mathbf{m}_s):\mathbf{b} - (\mathbf{m}_s\cdot\nabla_s)\cdot\nabla_s]\mathrm{d}A$$
$$+ \int_{\partial\Omega}\delta\mathbf{u}_s\cdot[\![2\mathbf{b}\cdot\mathbf{m}_s]\!]\cdot\mathbf{n}\mathrm{d}l - \int_{\partial\Omega}\delta u^n[\![\mathbf{m}_s\cdot\nabla_s]\!]\cdot\mathbf{n}\mathrm{d}l + \int_{\partial\Omega}(\delta u^n\nabla_s)\cdot[\![\mathbf{m}_s]\!]\cdot\mathbf{n}\mathrm{d}l \tag{73}$$

where $\mathrm{d}l$ is the element of the arc length on $\partial\Omega$, $\mathbf{n} = \mathbf{l}\times\boldsymbol{a}_3$, with $\boldsymbol{l}$ being the unit tangent vector of $\partial\Omega$. Likewise, the boundary integrals vanish in Eqs. (72) and (73) because the interface stress and the interface bending moment are continuous across the closed curve $\nabla_s$. Therefore substitute Eqs. (72) and (73) into Eq. (64), and we get

$$\int_{A_0}\delta(J_2\gamma)\mathrm{d}A_0 = \int_A\delta\mathbf{u}_s\cdot[-(\boldsymbol{\sigma}_s - \mathbf{b}\cdot\mathbf{m}_s)\cdot\nabla_s - \mathbf{b}\cdot(\mathbf{m}_s\cdot\nabla_s)]\mathrm{d}A$$
$$+ \int_A\delta u^n[-(\boldsymbol{\sigma}_s - \mathbf{b}\cdot\mathbf{m}_s):\mathbf{b} - (\mathbf{m}_s\cdot\nabla_s)\cdot\nabla_s]\mathrm{d}A \tag{74}$$

Next, the second term on the right side of Eq. (31) can be converted into the Eulerian description as follows by using Eq. (55)

$$\int_{v_0}\delta(\rho_0\psi_0)\mathrm{d}v_0 = \int_v\boldsymbol{\sigma}:(\delta\mathbf{u}\nabla)\mathrm{d}v = \int_{\partial v_T}\delta\mathbf{u}\cdot(\boldsymbol{\sigma}\cdot\mathbf{N})\mathrm{d}S - \int_A\delta\mathbf{u}\cdot[\![\boldsymbol{\sigma}]\!]\cdot\boldsymbol{a}_3\mathrm{d}A - \int_v\delta\mathbf{u}\cdot(\boldsymbol{\sigma}\cdot\nabla)\mathrm{d}v \tag{75}$$

where $\mathbf{N}$ is the unit normal vector to the boundary in the current configuration, and $[\![\boldsymbol{\sigma}]\!]$ represents the discontinuity of the Cauchy stress across the interface $A$.

Finally, the variation of the external potential energy on the right-hand side of Eq. (31) can also be converted into the following Eulerian description

$$-\int_{v_0}\delta\mathbf{u}\cdot(\rho_0\mathbf{f})\mathrm{d}v_0 - \int_{\partial v_{0T}}(\delta\mathbf{u}\cdot{}_0\bar{\mathbf{t}})\mathrm{d}s_0 = -\int_v\delta\mathbf{u}\cdot(\rho\mathbf{f})\mathrm{d}v - \int_{\partial v_T}(\delta\mathbf{u}\cdot\bar{\mathbf{t}})\mathrm{d}s \tag{76}$$

If one substitutes Eqs. (74)–(76) into Eq. (31) and considers the arbitrariness of $\delta\boldsymbol{u}$, the vanishing of the variation of the energy functional generates the following equations:

$$\boldsymbol{\sigma}\cdot\nabla + \rho\mathbf{f} = 0 \quad (\text{in } v)$$
$$\boldsymbol{\sigma}\cdot\mathbf{N} = \bar{\mathbf{t}} \qquad (\text{on } \partial v_T) \tag{77}$$

$$\boldsymbol{a}_3\cdot[\![\boldsymbol{\sigma}]\!]\cdot\boldsymbol{a}_3 = -(\boldsymbol{\sigma}_s - \mathbf{b}\cdot\mathbf{m}_s):\mathbf{b} - (\mathbf{m}_s\cdot\nabla_s)\cdot\nabla_s \quad (\text{on } A)$$
$$\mathbf{P}\cdot[\![\boldsymbol{\sigma}]\!]\cdot\boldsymbol{a}_3 = -(\boldsymbol{\sigma}_s - \mathbf{b}\cdot\mathbf{m}_s)\cdot\nabla_s + \mathbf{b}\cdot(\mathbf{m}_s\cdot\nabla_s) \quad (\text{on } A) \tag{78}$$

where $\mathbf{P} = \mathbf{I} - \boldsymbol{a}_3\otimes\boldsymbol{a}_3$. Obviously, Eq. (77) contains the well-known equilibrium equation and boundary condition from the classical theory of elasticity, while Eq. (78) is the Eulerian description of the generalized Young–Laplace equation. It is interesting to note that Eq. (78) can also be written is a compact form

$$[\![\boldsymbol{\sigma}]\!]\cdot\boldsymbol{a}_3 = -\boldsymbol{\Sigma}_s\cdot\tilde{\nabla}_s \tag{79}$$

where $\boldsymbol{\Sigma}_s = \boldsymbol{\sigma}_s - \mathbf{b}\cdot\mathbf{m}_s + \boldsymbol{a}_3\otimes(\mathbf{m}_s\cdot\nabla_s)$ is a combination of the interface stress and bending moment. It can be shown that $\boldsymbol{\Sigma}_s$ and Eq. (79) are equivalent to the equations (4.30) and (4.34), respectively, in Steigmann and Ogden (1999). However, in comparison, Eq. (78) shows explicitly the equilibrium features of the interface and the roles of the interface stress and bending moment.

It is worth noting that the explicit expressions of the generalized Young–Laplace equation under both Lagrangian and Eulerian descriptions are obtained in a unified scheme for the first time in this paper. Notably, the Lagrangian description is preferable when dealing with large elastic deformation of heterogeneous materials because, for such materials, the shapes of the deformed body and interfaces are generally unknown. Moreover, nano-structured materials are residually stressed at their initial state. It has been demonstrated in the literature (Sun et al., 2004; Huang and Sun, 2007; Gao et al., 2013) that only by utilizing the Lagrangian description of the fundamental equations for the interface can we properly and conveniently investigate the influence of residual interface stress/bending moment on the overall properties of nanostructures.

## 6. The determination of the residual elastic field

It has been stated that the residual field $\boldsymbol{\sigma}^*$ in the bulk does not vanish in the initial state because of the existence of interfacial energy. When the current configuration coincides with the reference configuration, the residual elastic field in

the bulk body satisfies the conventional equilibrium equations and boundary conditions:

$$\boldsymbol{\sigma}^* \cdot \nabla_0 = 0 \quad (\text{in } v_0)$$
$$\boldsymbol{\sigma}^* \cdot {}_0\mathbf{N} = 0 \quad (\text{on } \partial v_{0T}) \tag{80}$$

Eq. (80) indicates that the residual elastic field is in a state of self-equilibrium where no external load is applied at the boundary, regardless of the body force. Across the material interface, the residual stress field should also satisfy the generalized Young–Laplace equation

$$\mathbf{P}_0 \cdot \llbracket \boldsymbol{\sigma}^* \rrbracket \cdot \mathbf{A}_3 = -(\boldsymbol{\sigma}_s^* - \mathbf{B} \cdot \mathbf{m}_s^*) \cdot \nabla_{0s} + \mathbf{B} \cdot (\mathbf{m}_s^* \cdot \nabla_{0s}) \quad (\text{on } A_0) \tag{81}$$

$$\mathbf{A}_3 \cdot \llbracket \boldsymbol{\sigma}^* \rrbracket \cdot \mathbf{A}_3 = -(\boldsymbol{\sigma}_s^* - \mathbf{B} \cdot \mathbf{m}_s^*) : \mathbf{B} - (\mathbf{m}_s^* \cdot \nabla_{0s}) \cdot \nabla_{0s} \quad (\text{on } A_0) \tag{82}$$

where the residual interface stress and bending moment are given in Eqs. (25) and (26). The above Eqs. (80)–(82) consist of the set of basic equations that determines the residual elastic field in the bulk. It is obvious that the residual stress field depends not only on the geometry of the zero traction boundaries but also on the geometry and physical properties of the interface.

## 7. Examples and applications

In this part, two simple examples are illustrated to show the validity and significance of the newly developed theory.

### 7.1. A prediction of the size-dependence of the residual surface stress

Because of the curvature-dependence of the interfacial energy, the residual interface stress and residual interface bending moment are also curvature-dependent. For a special case, we consider a spherical nano-inhomogeneity or a spherical nanoparticle with radius $R$ in a heterogeneous material where the curvature tensor of the sphere is $\mathbf{B} = -\mathbf{i}_0/R$. Thus the residual interface stress and the residual interface bending moment reduce to

$$\boldsymbol{\sigma}_s^* = \left(\gamma_0 + 2\gamma_1 + 2\gamma_2 + \frac{2\gamma_5}{R}\right)\mathbf{i}_0 \tag{83}$$

$$\mathbf{m}_s^* = \left(\gamma_3 + \gamma_5 + \frac{\gamma_4}{R}\right)\mathbf{i}_0 \tag{84}$$

which demonstrate that the curvature-dependence has implications for size-dependence. The spherical surface has a constant curvature thus Eqs. (83) and (84) are both isotropic. If we set $\gamma_0^* = \gamma_0 + 2\gamma_1 + 2\gamma_2$ and omit the unit tensor $\mathbf{i}_0$ in Eq. (83), we obtain

$$\sigma_s^* = \gamma_0^* + \frac{2\gamma_5}{R} \tag{85}$$

which is different from the conventional residual surface/interface stress existing in the literature (e.g., Gurtin and Murdoch, 1975, 1978; Huang and Wang, 2013). The first term on the right side of Eq. (85) represents the constant part of the residual surface/interface stress which is consistent with classical results. The second term on the right side of Eq. (85), however, represents the curvature-dependent part of the residual surface/interface stress which is newly developed in this study.

Results from many theoretical, experimental and computational studies support the size-dependence of surface/interfacial energy and surface/interface stress (e.g., Tolman, 1949; Jiang and Lu, 2008; Medasani and Vasiliev, 2009). One of the most important findings appears in the famous Tolman's formula which describes the size effect of the residual surface stress and gives

$$\sigma_s = \sigma_\infty \left(1 + \frac{2\delta_\infty}{R}\right)^{-1} \tag{86}$$

where $\sigma_s$ denotes the residual surface stress of a spherical surface, $\sigma_\infty$ denotes the residual surface stress of a planar surface and $\delta_\infty$ is the well-known Tolman length. If one takes a Taylor series expansion of Eq. (86) with variable $R$ and keeps to the first non-constant term (Schmelzer, 1986), the Tolman's formula can be approximately written as

$$\sigma_s = \sigma_\infty \left(1 - \frac{2\delta_\infty}{R}\right) + O(R^{-2}) \tag{87}$$

This approximate formula works in the range $R/\delta_\infty \geq 10$ (Lu and Jiang, 2005).

If one compares Eq. (85) given by the present theory with the approximate Tolman's formula Eq. (87), one may then find that these two equations coincide with each other and that the parameters have the following corresponding relations

$$\sigma_\infty = \gamma_0^*, \; \delta_\infty = -\gamma_5/\gamma_0^* \tag{88}$$

which indicate that the constant part $\gamma_0^*$ in Eq. (85) represents the residual surface stress of a planar surface and $\gamma_5$ is associated with the Tolman length.

In addition, the size-dependence of residual surface stress predicted by the present theory is also in good agreement with results for aluminum (Al) nanoparticles calculated by molecular dynamics and *ab initio* (Medasani and Vasiliev, 2009) shown in Fig. 2. The colored lines denote the fitting curves by Tolman's formula and the present theory. For the Tolman's formula in Eq. (86), the fitting parameters are $\sigma_\infty = 2.3$ N/m and $\delta_\infty = 1.26 \times 10^{-10}$ m, while for our predicting formula in Eq. (85), the fitting parameters $\gamma_0^* = 2.18$ N/m and $\gamma_5 = -1.46 \times 10^{-10}$ N. Fig. 2 illustrates the facts that both the fitting curves can well capture the size-dependence of the residual surface stress, and furthermore, that the results predicted by Tolman's formula and the present theory are very closed to each other, thus reflecting the validity of the present theory.

### 7.2. The residual field in an infinite matrix with spherical voids

In this section, we discuss the effect of the curvature-dependent surface energy on the residual elastic field for hyperelastic materials. As an example, we consider the case shown in Fig. 3 which describes a spherical void embedded in an infinite hyperelastic matrix. Assuming the matrix is a harmonic material introduced by John (1960), its corresponding hyperelastic potential is

$$\rho_0 \psi_0 = f(i_1) + c_2(i_2 - 3) + c_3(i_3 - 1), f''(i_1) \neq 0 \tag{89}$$

where $f$ is function of its indicated argument, $c_2$ and $c_3$ are material constants, and $i_1$, $i_2$, $i_3$ are principal invariants of the stretch tensor $\tilde{\mathbf{U}} = \tilde{\mathbf{C}}^{1/2}$, that are defined as follows: $i_1 = \lambda_1 + \lambda_2 + \lambda_3$, $i_2 = \lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1$ and $i_3 = \lambda_1\lambda_2\lambda_3$.

It is usually required that restrictions be imposed on the hyperelastic potential. These restrictions are as follows: (i) in the fictitious stress-free configuration, the hyperelastic potential and the stress field vanish; and (ii) in the case of infinitesimal deformations, the hyperelastic potential function should reduce to the classical linear elasticity theory. According to the above restrictions, for the harmonic material, we obtain

$$f(3) = 0, f'(3) = -2c_2 - c_3, c_2 + c_3 = -2\mu < 0, f''(3) = K + \frac{4}{3}\mu \tag{90}$$

where $\mu$ is the shear modulus and $K$ is the bulk modulus of linear elastic materials.
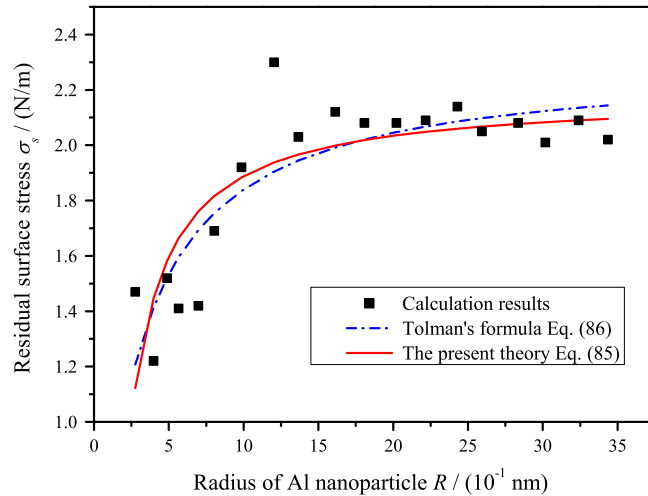


**Fig. 2.** The size-dependence of the residual surface stress of Al nanoparticles. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
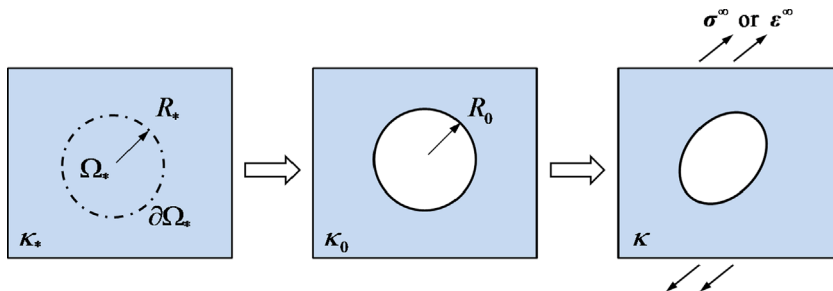


**Fig. 3.** The three configurations in the developed interface stress theory.

What we are concerned with is the residual elastic field in the reference configuration $\kappa_0$. As illustrated in Fig. 3, in the fictitious stress-free configuration $\kappa_*$, a spherical part $\Omega_*$ with radius $R_*$ is taken out from the bulk solid. Then the atoms on the newly created surface will move to new equilibrium positions and induce a residual elastic field in the bulk solid. For the problem we are investigating, the deformation from $\kappa_*$ to $\kappa_0$ is spherically symmetric and can be described by $r = r(R)$, $\theta = \Theta$ and $\phi = \Phi$, where $(R, \Theta, \Phi)$ and $(r, \theta, \phi)$ denote spherical polar coordinates before and after deformation, with the principal stretches being

$$\lambda_1 = \frac{dr(R)}{dR} = r', \quad \lambda_2 = \lambda_3 = \frac{r(R)}{R} (R \geq R_*) \tag{91}$$

The radial and hoop components of the Cauchy stress $\sigma$ can be expressed in terms of hyperelastic potential as follows:

$$\sigma_r = \rho_0 \frac{1}{\lambda_2^2} \frac{\partial \psi_0}{\partial \lambda_1}, \sigma_\theta = \sigma_\phi = \rho_0 \frac{1}{\lambda_1 \lambda_2} \frac{\partial \psi_0}{\partial \lambda_2} \tag{92}$$

Hence, the equilibrium equation in the absence of body force can be written as

$$\frac{d}{dR}\left(R^2 \frac{\partial \psi_0}{\partial \lambda_1}\right) - 2R \frac{\partial \psi_0}{\partial \lambda_2} = 0 \tag{93}$$

For the harmonic material, the solution of Eq. (93) is

$$r(R) = k_1 R + \frac{k_2}{R^2} \tag{94}$$

The key to this residual field problem is how to determine the radius $R_0 = r(R_*)$ of the newly formed spherical void in the initial reference configuration.

Considering the remote field conditions that $\lambda_1$ and $\lambda_2$ converge to 1 at infinity, we obtain $k_1 = 1$ and $i_1 = 3k_1 = 3$. Hence, $\sigma_r$ in Eq. (92) can be written as

$$\sigma_r = \left(\frac{1}{\lambda_2}\right)^2 [f'(3) + 2c_2\lambda_2 + c_3\lambda_2^2] = \left(\frac{1}{\lambda_2}\right)^2 [2c_2(\lambda_2 - 1) + c_3(\lambda_2^2 - 1)] \tag{95}$$

By using the generalized Young–Laplace Eqs. (81) and (82) on $r = r(R_*) = R_0$ in the reference configuration and noting that Eq. (81) is automatically satisfied, we get

$$\sigma_r|_{r=r(R_*)} = \frac{2}{R}\left[\left(\gamma_0^* + \frac{2\gamma_5}{R}\right) + \left(\gamma_3 + \gamma_5 + \frac{\gamma_4}{R}\right)\frac{1}{R}\right] = 2\left(\frac{\gamma_0^*}{R} + \frac{\gamma_3 + 3\gamma_5}{R^2} + \frac{\gamma_4}{R^3}\right) \tag{96}$$

If we then substitute Eq. (95) into Eq. (96), we arrive at

$$c_3\lambda_*^3 + 2\left(c_2 - \frac{\gamma_0^*}{R_*}\right)\lambda_*^2 - \left(\frac{2(\gamma_3 + 3\gamma_5)}{R_*^2} + (2c_2 + c_3)\right)\lambda_* - \frac{2\gamma_4}{R_*^3} = 0 \tag{97}$$

where

$$\lambda_* = \frac{r(R_*)}{R_*} = \frac{R_0}{R_*} = 1 + \frac{k_2}{R_*^3} > 0 \tag{98}$$

If $R_*$ is known in advance, Eq. (97) will determine $\lambda_*$ and then $k_2$ can be determined from Eq. (98). Once the deformation relation in Eq. (94) is determined, we can immediately obtain the residual stress field in the reference configuration. It is worth noting that Eq. (97) will reduce to the results of Huang and Wang (2006) if we neglect the residual surface bending moment and the curvature-dependent part of the residual surface stress by setting $\gamma_3 = \gamma_4 = \gamma_5 = 0$.

For simplicity, we only consider the effect of the curvature-dependent residual surface stress. Hence, Eq. (97) reduces to a quadratic equation

$$c_3\lambda_*^2 + 2\left(c_2 - \frac{\gamma_0^*}{R_*}\right)\lambda_* - \left(\frac{4\gamma_5}{R_*^2} + (2c_2 + c_3)\right) = 0 \tag{99}$$

Therefore, we can solve for $\lambda_*$:

$$\lambda_* = \begin{cases} -\left(\frac{c_2}{c_3} - \frac{\gamma_0^*}{c_3 R_*}\right) + \sqrt{\left(\frac{c_2}{c_3} - \frac{\gamma_0^*}{c_3 R_*}\right)^2 + \left(1 + \frac{2c_2}{c_3} + \frac{4\gamma_5}{R_*^2}\right)} & \text{if } c_3 < 0 \\ -\left(\frac{c_2}{c_3} - \frac{\gamma_0^*}{c_3 R_*}\right) - \sqrt{\left(\frac{c_2}{c_3} - \frac{\gamma_0^*}{c_3 R_*}\right)^2 + \left(1 + \frac{2c_2}{c_3} + \frac{4\gamma_5}{R_*^2}\right)} & \text{if } c_3 > 0 \end{cases} \tag{100}$$

In particular, if $\gamma_0^*/(c_3 R_*)$ and $\gamma_5/(c_3 R_*^2)$ (as compared with unity) are first order small quantities and high-order small quantities are neglected, then the approximate values of $\lambda_*$ and $k_2$ are

$$\lambda_* = 1 - \frac{1}{2\mu R_*}\left(\gamma_0^* + \frac{2\gamma_5}{R_*}\right), \quad k_2 = -\frac{R_*^2}{2\mu}\left(\gamma_0^* + \frac{2\gamma_5}{R_*}\right) \tag{101}$$

Then the radial stress and hoop stress are obtained as

$$\sigma_r = \mu H \cdot \frac{4k^3 + c_3 H/\mu}{(k^3 - H)^2}, \quad \sigma_\theta = \sigma_\phi = -2\mu H \cdot \frac{k^3 + c_3 H/\mu}{(k^3 + 2H)(k^3 - H)} \tag{102}$$

where

$$H = \frac{1}{2\mu R_*}\left(\gamma_0^* + \frac{2\gamma_5}{R_*}\right), \quad k = \frac{R}{R_*} \geq 1 \tag{103}$$

Here we note that $H$ is a parameter that reflects the surface effect. It is obvious that two intrinsic length scales, $l_s = \gamma_0^*/\mu$ and $k_s = -\gamma_5/\gamma_0^*$, emerge in Eq. (103), so that

$$H = \frac{l_s}{2R_*} \cdot \left(1 - 2\frac{k_s}{R_*}\right) \tag{104}$$

It is seen from Eq. (88) that $l_s$ reflects the effect of the constant part of the residual surface stress, which has been extensively used in the classical surface stress theory, while $k_s$ is a new intrinsic length scale brought up in the present theory, which approximately equals to the Tolman length and is associated with the curvature-dependence of the residual surface stress. Hence, a dimensionless parameter can be introduced to estimate the importance of the curvature-dependent part of the residual surface stress relative to its constant part:

$$k_r = \frac{k_s}{l_s} = -\frac{\mu\gamma_5}{(\gamma_0^*)^2} \doteq \frac{\mu\delta_\infty}{\gamma_0^*} \tag{105}$$
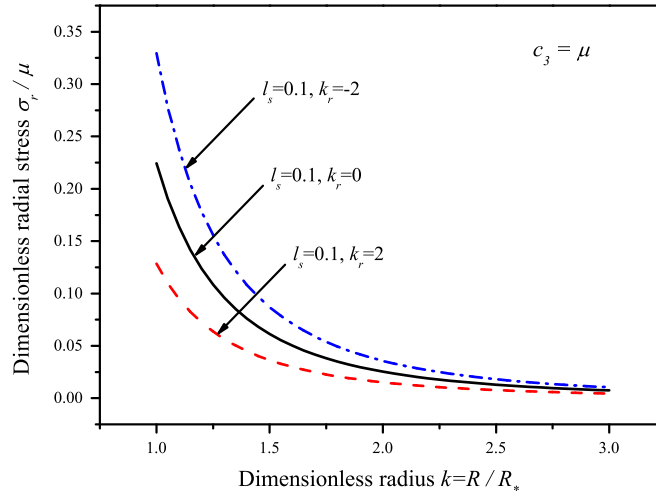


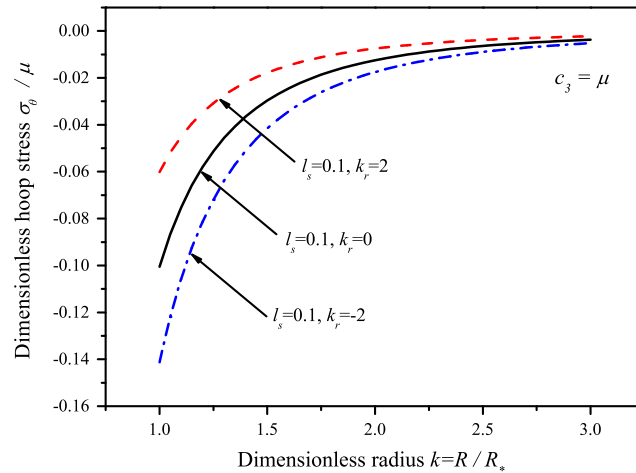**Fig. 4.** The distribution of the radial residual stress.



**Fig. 5.** The distribution of the hoop residual stress.

For the Al nanoparticle investigated in Section 7.1, the dimensionless parameter $k_r$ is about 0.82 (the shear modulus of Al is 26.56 GPa).

The distributions of the radial and hoop stresses are illustrated in Figs. 4 and 5 where it is assumed that $c_3 = \mu$ and the dimensionless surface parameters have the following values: $l_s/R_* = 0.1$ and $k_r = \pm 2$. It is shown that the curvature-dependence of residual surface stress does have a significant influence on the distributions of the residual elastic field in the bulk.

## 8. Conclusions

In the present paper, a curvature-dependent interfacial energy-based interface stress theory is developed. This theory is formulated within the framework of continuum mechanics and therefore valid for large elastic deformation problems of heterogeneous nano-materials. The significance and the originality of this work are as follows:

1. The fundamental equations for the interface were derived in Lagrangian description, which are advantageous for modeling the effects of residual interface stress, residual interface bending moment and interface elasticity on the effective properties of nanomaterials.
2. A new nonlinear constitutive relation of the interface has been formulated based on the curvature-dependent interfacial energy. This constitutive relation explicitly demonstrates the curvature-dependent nature of the interface stress and bending moment, which is different from that described by the classical theories.
3. A new energy functional for heterogeneous hyperelastic solids with interfaces is proposed. Both the Lagrangian and Eulerian descriptions of the generalized Young–Laplace equation have been derived firstly from this energy functional. The newly derived generalized Young–Laplace equation can describe the intrinsic flexural resistance of the material interface.
4. The concept and importance of the residual elastic field induced by the interfacial energy are elucidated in this paper. Utilizing this newly developed theory, this paper then provides a set of basic equations for determining the residual elastic field in heterogeneous media containing interfaces.
5. Two examples are presented in order to shed light on the significance of the present theory. The first example shows that our theory is capable of accounting for the size-dependence of the residual surface stress of spherical nanoparticles, which is in agreement with the Tolman's formula and the relevant results in the literature. The second example demonstrates that the curvature-dependence of the residual surface stress may have a significant influence on the residual stress field in the elastic body. A new dimensionless intrinsic parameter is suggested to characterize the importance of the curvature-dependent part of the residual surface stress.

## Appendix A. The Lagrangian description of the normal vector $a_3$

Considering Eq. (1), we have

$$\boldsymbol{a}_\alpha = X_\alpha^\lambda \mathbf{A}_\lambda + D_\alpha \mathbf{A}_3 \tag{A.1}$$

where $X_\alpha^\lambda = \delta_\alpha^\lambda + u_0^\lambda|_\alpha - u_0^n B_\alpha^\lambda$ and $D_\alpha = u_0^\lambda B_{\lambda\alpha} + u_{0,\alpha}^n$. Substituting (A.1) into $\boldsymbol{a}_3 = 1/2\mu^{\alpha\beta}\boldsymbol{a}_\alpha \otimes \boldsymbol{a}_\beta$ and after simple algebra calculations, we can finally get

$$\boldsymbol{a}_3 = \frac{1}{J_2}\left(X\mathbf{A}_3 - \boldsymbol{\varepsilon}^{\mathrm{T}} \cdot \mathbf{F}_s^{(in)} \cdot \boldsymbol{\varepsilon} \cdot \mathbf{D}\right) = \frac{1}{J_2}(X\mathbf{A}_3 - \mathbf{Z}) \tag{A.2}$$

where $X = \det(X_\alpha^\lambda) = \det \mathbf{F}_s^{(in)}$ and

$$\mathbf{Z} = Z_\gamma \mathbf{A}^\gamma = \boldsymbol{\varepsilon}^{\mathrm{T}} \cdot \mathbf{F}_s^{(in)} \cdot \boldsymbol{\varepsilon} \cdot \mathbf{D}, Z_\gamma = \varepsilon^{\alpha\beta}\varepsilon_{\mu\gamma}X_\alpha^\mu D_\beta \tag{A.3}$$

## Appendix B. The variation of $Z$, $J_2$ and $X$

(i) Considering (A.3), we have

$$\delta\mathbf{Z} = \delta Z_\gamma \mathbf{A}^\gamma = \varepsilon^{\alpha\beta}\varepsilon_{\mu\gamma}(\delta X_\alpha^\mu D_\beta + X_\alpha^\mu \delta D_\beta)\mathbf{A}^\gamma \tag{B.1}$$

Thus, we have

$$\delta \mathbf{Z} = \boldsymbol{\varepsilon}^{\mathrm{T}} \cdot \delta \mathbf{F}_s^{(in)} \cdot \boldsymbol{\varepsilon} \cdot \mathbf{D} + \boldsymbol{\varepsilon}^{\mathrm{T}} \cdot \mathbf{F}_s^{(in)} \cdot \boldsymbol{\varepsilon} \cdot \delta \mathbf{D} \tag{B.2}$$

It is noted that $\boldsymbol{\varepsilon}^{\mathrm{T}} \cdot \mathbf{F}_s^{(in)} \cdot \boldsymbol{\varepsilon} = (\mathrm{tr}\mathbf{F}_s^{(in)})\mathbf{i}_0 - (\mathbf{F}_s^{(in)})^{\mathrm{T}}$.

(ii) Considering $J_2 = \sqrt{I_2}$ and $I_2 = 1/2(I_1^2 - \mathrm{tr}\mathbf{C}_s^2)$, we have

$$\delta J_2 = \frac{1}{2J_2} \delta I_2 = \frac{1}{2J_2} (I_1 \mathbf{i}_0 - \mathbf{C}_s) : \ \delta \mathbf{C}_s \tag{B.3}$$

(iii) Considering $X = \det \mathbf{F}_s^{(in)} = 1/2[(\mathrm{tr}\mathbf{F}_s^{(in)})^2 - \mathrm{tr}(\mathbf{F}_s^{(in)})^2]$, we get

$$\delta X = [(\mathrm{tr}\mathbf{F}_s^{(in)})\mathbf{i}_0 - (\mathbf{F}_s^{(in)})^{\mathrm{T}}] : \ \delta \mathbf{F}_s^{(in)} \tag{B.4}$$

## References

Angenent, S., Gurtin, M.E., 1989. Multiphase thermodynamics with interfacial structure 2. Evolution of an isothermal interface. Arch. Ration. Mech. Anal. 108 (4), 323–391.

Cahn, J.W., 1978. Thermodynamics of solid and fluid surfaces. In: Johnson, W.C., Blakely, J.M. (Eds.), Interfacial Segregation. American Society for Metals, Metals Park, OH, pp. 3–23.

Cammarata, R.C., 1994. Surface and interface stress effects in thin films. Prog. Surf. Sci. 46 (1), 1–38.

Chen, C.Q., Shi, Y., Zhang, Y.S., Zhu, J., Yan, Y.J., 2006. Size dependence of Young's modulus of ZnO nanowires. Phys. Rev. Lett. 96 (7), 075505.

Chhapadia, P., Mohammadi, P., Sharma, P., 2011. Curvature-dependent surface energy and implications for nanostructures. J. Mech. Phys. Solids 59 (10), 2103–2115.

Das, S.K., Binder, K., 2011. Universal critical behavior of curvature-dependent interfacial tension. Phys. Rev. Lett. 107 (23), 235702.

Dingreville, R., Qu, J., Cherkaoui, M., 2005. Surface free energy and its effect on the elastic behavior of nano-sized particles, wires and films. J. Mech. Phys. Solids 53 (8), 1827–1854.

Dingreville, R., Qu, J., 2008. Interfacial excess energy, excess stress and excess strain in elastic solids: Planar interfaces. J. Mech. Phys. Solids 56 (5), 1944–1954.

Duan, H.L., Wang, J., Huang, Z.P., Karihaloo, B.L., 2005a. Size-dependent effective elastic constants of solids containing nano-inhomogeneities with interface stress. J. Mech. Phys. Solids 53 (7), 1574–1596.

Duan, H.L., Wang, J., Huang, Z.P., Karihaloo, B.L., 2005b. Eshelby formalism for nano-inhomogeneities. Proc. R. Soc. A 461 (2062), 3335–3353.

Gao, X., Hao, F., Fang, D.N., Huang, Z.P., 2013. Boussinesq problem with the surface effect and its application to contact mechanics at the nanoscale. Int. J. Solids Struct. 50 (16-17), 2620–2630.

Ghahremani, F., 1980. Effect of grain-boundary sliding on anelasticity polycrystals. Int. J. Solids Struct. 16 (9), 825–845.

Gibbs, J.W., 1906. The Scientific Papers of J. Willard Gibbs, vol 1. Longmans-Green, London.

Green, A.E., Zerna, W., 1960. Theoretical Elasticity. Oxford University Press, London.

Gurtin, M.E., Murdoch, A.I., 1975. A continuum theory of elastic material surfaces. Arch. Ration. Mech. Anal. 57 (4), 291–323.

Gurtin, M.E., Murdoch, A.I., 1978. Surface stress in solids. Int. J. Solids Struct. 14 (6), 431–440.

Gurtin, M.E., 1988. Multiphase thermodynamics with interfacial structure 1. Heat conduction and the capillary balance law. Arch. Ration. Mech. Anal. 112 (2), 97–160.

Gurtin, M.E., Struthers, A., 1990. Multiphase thermodynamics with interfacial structure 3. Evolving phase boundaries in the presence of bulk deformation. Arch. Ration. Mech. Anal. 104 (3), 195–221.

Gurtin, M.E., Weissmuller, J., Larche, F., 1998. A general theory of curved deformable interfaces in solids at equilibrium. Philos. Mag. A 78 (5), 1093–1109.

Hashin, Z., 1991a. The spherical inclusion with imperfect interface. J. Appl. Mech. 58 (2), 444–449.

Hashin, Z., 1991b. Thermoelastic properties of particulate composites with imperfect interface. J. Mech. Phys. Solids 39 (6), 745–762.

He, L.H., Lim, C.W., Wu, B.S., 2004. A continuum model for size-dependent deformation of elastic films of nano-scale thickness. Int. J. Solids Struct. 41 (3–4), 847–857.

He, L.H., Li, Z.R., 2006. Impact of surface stress on stress concentration. Int. J. Solids Struct. 43 (20), 6209–8219.

Helfrich, W., 1973. Elastic properties of lipid bilayers: theory and possible experiments. Z. Naturforsch. C 28 (11-1), 693–703.

Herring, C., 1951. Surface tension as a motivation for sintering. In: Kingston, W.E. (Ed.), The Physics of Power Metallurgy. McGraw Hill, New York, pp. 143–179.

Herring, C., 1953. The use of classical macroscopic concepts in surface energy problems. In: Gomer, R., Smith, C.S. (Eds.), Structure and Properties of Solid Surface. The University of Chicago press, Chicago, pp. 5–81.

Hoger, A., 1986. On the determination of residual stress in an elastic body. J. Elasticity 16 (3), 303–324.

Hoger, A., 1993. The elasticity tensors of a residually stressed material. J. Elasticity 31 (3), 219–237.

Huang, J.H., Furuhashi, R., Mura, T., 1993. Frictional sliding inclusions. J. Mech. Phys. Solids 41 (2), 247–265.

Huang, Z.P., Wang, J., 2006. A theory of hyperelasticity of multi-phase media with surface/interface energy effect. Acta Mech. 182 (3-4), 195–210. (Erratum: Acta Mech. 215 (1–4), 365–366).

Huang, Z.P., Sun, L., 2007. Size-dependent effective properties of a heterogeneous material with interface energy effect: from finite deformation theory to infinitesimal strain analysis. Acta Mech. 190 (1–4), 151–163. Erratum: Acta Mech. 215 (1–4), 363–364.

Huang, Z.P., 2012. Fundamentals of Continuum Mechanics, second ed. Higher Education Press, Beijing (In Chinese).

Huang, Z.P., Wang, J., 2013. Micromechanics of nanocomposites with interface energy effect. In: Li, S.F., Gao, X.L. (Eds.), Handbook of Micromechanics and Nanomechanics. Pan Stanford Publishing Pte. Ltd., Singapore, pp. 303–348.

Jiang, Q., Zhao, D.S., Zhao, M., 2001. Size-dependent interface energy and related interface stress. Acta Mater. 49 (16), 3134–3147.

Jiang, Q., Lu, H.M., 2008. Size dependent interface energy and its applications. Surf. Sci. Rep. 63 (10), 427–464.

Jing, G.Y., Duan, H.L., Sun, X.M., Zhang, Z.S., Xu, J., Li, Y.D., Wang, J.X., Yu, D.P., 2006. Surface effects on elastic properties of silver nanowires: Contact atomic-force microscopy. Phys. Rev. B 73 (23), 235409.

John, F., 1960. Plane strain problems for a perfectly elastic material of harmonic type. Commun. Pure Appl. Math. 13 (2), 239–296.

Langhaar, H.L., 1974. Elastic surfaces and theories of shells. Acta Mech. 19 (1-2), 109–128.

Lei, Y.A., Bykov, T., Yoo, S., Zeng, X.C., 2005. The Tolman length: Is it positive or negative? J. Am. Chem. 127 (44), 15346–15347.

Lu, H.M., Jiang, Q., 2004. Size-dependent surface energies of nanocrystals. J. Phys. Chem. B 108 (18), 5617–5619.

Lu, H.M., Jiang, Q., 2005. Size-dependent surface energies of nanocrystals. Langmuir 21 (2), 779–781.

Medasani, B., Park, Y.H., Vasiliev, I., 2007. Theoretical study of the surface energy, stress, and lattice contraction of silver nanoparticles. Phys. Rev. B 75 (23), 235436.

Medasani, B., Vasiliev, I., 2009. Computational study of the surface properties of aluminum nanoparticles. Surf. Sci. 603 (13), 2042–2046.

Mi, C.W., Kouris, D., 2012. On the significance of the coherent interface effects on the embedded nanoparticles. Math. Mech. Solids http://dx.doi.org/10.1177/1081286512465426. (e-pubulication).

Miller, R.E., Shenoy, V.B., 2000. Size-dependent elastic properties of nanosized structural elements. Nanotechnology 11 (3), 139–147.

Mohammadi, P., Sharma, P., 2012. Atomistic elucidation of the effect of surface roughness on curvature-dependent surface energy, surface stress, and elasticity. Appl. Phys. Lett. 100 (13), 133110.

Murr, L.E., 1975. Interfacial Phenomena in Metals and Alloys. Addison-Wesley, London.

Mura, T., Furuhashi, R., 1984. The elastic inclusion with a sliding interface. J. Appl. Mech. 51 (2), 308–310.

Mura, T., Jasiuk, I., Tsuchida, E., 1985. The stress field of a sliding inclusion. Int. J. Solids Struct. 21 (12), 1165–1179.

Nanda, K.K., 2012. Liquid-drop model for the surface energy of nanoparticles. Phys. Lett. A 376 (19), 1647–1649.

Ou-Yang, Z.C., Helfrich, W., 1987. Instability and deformation of a spherical vesicle by pressure. Phys. Rev. Lett. 59 (21), 2486–2488.

Orowan, E., 1970. Surface energy and surface tension in solids and liquids. Proc. R. Soc. Lond. A 316 (1527), 472–491.

Park, H.S., Klein, P.A., 2008. Surface stress effects on the resonant properties of metal nanowires: The importance of finite deformation kinematics and the impact of the residual surface stress. J. Mech. Phys. Solids 56 (11), 3144–3166.

Povstenko, Y.Z., 1993. Theoretical investigation of phenomena caused by heterogeneous surface tension in solids. J. Mech. Phys. Solids 41 (9), 1499–1514.

Qu, J.M., 1993. The effect of slightly weakened interfaces on the overall elastic properties of composite-materials. Mech. Mater. 14 (4), 269–281.

Schmelzer, J., 1986. The curvature dependence of surface tension of small droplets. J. Chem. Soc., Faraday Trans. 1 (82), 1421–1428.

Seth, B.R., 1964. Generalized strain measures with application to physical problems. In: Reiner, M., Abir, D. (Eds.), Second-Order Effects in Elasticity, Plasticity and Fluid Dynamics. Pergamon Press, Oxford, pp. 162–172.

Sharma, P., Ganti, S., Bhate, N., 2003. Effect of surfaces on the size-dependent elastic state of nano-inhomogeneities. Appl. Phys. Lett. 82 (4), 535–537.

Sharma, P., Ganti, S., 2004. Size-dependent Eshelby's tensor for embedded nano-inclusions incorporating surface/interface energies. J. Appl. Mech. 71 (5), 663–671.

Sharma, P., Wheeler, L.T., 2007. Size-dependent elastic state of ellipsoidal nano-inclusions incorporating surface/interface tension. J. Appl. Mech. 74 (3), 447–454.

Shen, H., Schiavone, P., Ru, C.Q., Mioduchowski, A., 2000. Analysis of internal stress in an elliptic inclusion with imperfect interface in plane elasticity. Math. Mech. Solids 5 (4), 501–521.

Shuttleworth, R., 1950. The surface tension of solids. Proc. Phys. Soc. A 63 (365), 444–457.

Steigmann, D.J., Ogden, R.W., 1999. Elastic surface-substrate interactions. Proc. R. Soc. Lond. A 455 (1982), 437–474.

Steigmann, D.J., 2001. Elements of the theory of the elastic surface. In: Fu, Y.B., Ogden, R.W. (Eds.), Nonlinear Elasticity: Theory and Application. Cambridge University Press, Cambridge, pp. 268–304.

Streitz, F.H., Cammarata, R.C., Sieradzki, K., 1994a. Surface-stress effects on elastic properties. I. Thin metal films. Phys. Rev. B 49 (15), 10699.

Streitz, F.H., Cammarata, R.C., Sieradzki, K., 1994b. Surface-stress effects on elastic properties. II. Metallic multilayers. Phys. Rev. B 49 (15), 10707.

Sun, C.Q., Wang, Y., Tay, B.K., Li, S., Huang, H., Zhang, Y.B., 2002. Correlation between the melting point of a nanosolid and the cohesive energy of a surface atom. J. Phys. Chem. B 106 (41), 10701–10705.

Sun, L., Wu, Y.M., Huang, Z.P., Wang, J.X., 2004. Interface effect on the effective bulk modulus of a particle-reinforced composite. Acta Mech. Sin. 20 (6), 676–679.

Tolman, R.C., 1949. The effect of droplet size on surface tension. J. Chem. Phys. 17 (3), 333–337.

Weissmuller, J., Cahn, J.W., 1997. Mean stresses in microstructures due to interface stresses: a generalization of a capillary equation for solids. Acta Mater. 45 (5), 1899–1906.

Zhang, Z., Huang, Z.P., 2004. The stress field of a spherical inhomogeneity with imperfect interface. In: Guo, Y.M., Chen, D.H., Tao, W.M. (Eds.), Proceedings of International Conference on Fracture and Damage of Advanced Materials. China Machine Press, Beijing, pp. 49–56.

Zhang, W.X., Wang, T.J., Chen, X., 2010. Effect of interface/surface stress on the plastic deformation of nanoporous materials and nanocomposites. Int. J. Plasticity 26 (7), 957–975.

Zheng, Q.S., 1993. Two-dimensional tensor function representation for all kinds of material symmetry. Proc. R. Soc. Lond. A 443 (1917), 127–138.

Zhong, Z., Meguid, S.A., 1997. On the elastic field of a spherical inhomogeneity with an imperfectly bonded interface. J. Elasticity 46 (2), 91–113.

Zhong, Z., Meguid, S.A., 1999. On the imperfectly bonded spherical inclusion problem. J. Appl. Mech. 66 (4), 839–846.