International Journal of Engineering Science 48 (2010) 140–150

Contents lists available at ScienceDirect

International Journal of Engineering Science

journal homepage: www.elsevier.com/locate/ijengsci

The effects of surface tension on the elastic properties of nano structures

Zhi-Qiao Wang [a], Ya-Pu Zhao [a,*], Zhu-Ping Huang [b]

[a] State Key Laboratory of Nonlinear Mechanics, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China
[b] LTCS and Department of Mechanics and Aerospace Engineering, College of Engineering, Peking University, Beijing 100871, China

ARTICLE INFO

Article history:
Received 3 April 2009
Received in revised form 9 July 2009
Accepted 21 July 2009
Available online 19 August 2009

Communicated by K.R. Rajagopal

Keywords:
Surface stress
Surface tension
Pure bending of nanowires
Aspect ratio

ABSTRACT

In the absence of external loading, surface tension will induce a residual stress field in the bulk of nano structures. However, in the prediction of mechanical properties of nano structures, the elastic response of the bulk is usually described by classical Hooke's law, in which the aforementioned residual stress was neglected in the existing literatures. The present paper investigates the influences of surface tension and the residual stress in the bulk induced by the surface tension on the elastic properties of nano structures. We firstly present the surface elasticity in the Lagrangian and the Eulerian descriptions and point out that even in the case of infinitesimal deformations the reference and the current configurations should be discriminated; otherwise the out-plane terms of surface displacement gradient, associated with the surface tension, may sometimes be overlooked in the Eulerian descriptions, particularly for curved and rotated surfaces. Then, the residual stress in the bulk is studied through the non-classical boundary conditions and used to construct the linear elastic constitutive relations for the bulk material. Finally, these relations are adopted to analyze the size-dependent properties of pure bending of Al nanowires. The present results show that surface tension will considerably affect the effective Young's modulus of Al nanowires, which decrease with either the decrease of nanowires thickness or the increase of the aspect ratio.

1. Introduction

The surface is a region with its own atom arrangement and properties differing from the bulk of materials [1]. Within the surface zone, all physical properties like density, energy and stress vary quickly along the direction of thickness. In the thermodynamics of surfaces, such a thin region is often modeled, as done by Gibbs [2], as a bidimensional geometrical boundary of bulk phases which extend uniformly right up to the mathematical surface. In order to preserve the total physical properties of the system, the excess physical properties have to be assigned to the geometrical surface. The concepts of surface excess energy and surface excess stress have been widely used in the communities of physics [1] and materials science [3,4].

For the surface of solid, Gibbs [2] pointed out that surface energy and surface stress are not identical; meaning that, a different amount of reversible work is required to form a unit surface than to increase a large surface by unit area through reversibly stretching it. Shuttleworth [5] derived the relations between surface stress and surface strain for small deformations, which were interpretated from an atomistic viewpoint [6]. Gurtin and Murdoch [7,8] established the theoretical framework of the surface elasticity under the classical theory of membrane. Steigmann and Ogden [9,10] generalized the Gurtin–Murdoch theory to incorporate flexural stiffness of the free surface directly into the constitutive response of surface. Dingreville and Qu [11] investigated the influence of Poisson's ratio effect on the surface properties under general loading conditions. Considering the stationary condition of energy functional, Huang et al. [12,13] proposed a hyperelastic surface

* Corresponding author.
E-mail address: yzhao@imech.ac.cn (Y.-P. Zhao).

0020-7225/$ - see front matter © 2009 Elsevier Ltd. All rights reserved.
doi:10.1016/j.ijengsci.2009.07.007

model both in the Lagrangian and in the Eulerian descriptions within the framework of finite deformations. For nano structured materials, due to the increasing surface-to-volume ratio, surface effects become predominant and can significantly modify the macroscopic properties of materials. Obviously, the size-dependent mechanical properties of nano structured materials can be modeled by continuum mechanics including the above-mentioned surface elasticity [14–20]. It will be shown that, even in the case of infinitesimal deformations, we should distinguish between the reference and the current configurations; otherwise the out-plane terms of surface displacement gradient, associated with the surface tension, may sometimes be overlooked in the Eulerian descriptions, particularly for curved and rotated surfaces.

In the absence of external loading, the surfaces of a nano structure will be subjected to residual surface stress, namely the surface tension. Thus, from generalized Young-Laplace equations, it can be concluded that the presence of surface tension manifests itself in a nonclassical boundary condition giving the force in the bulk of nano structures to equilibrate the surface tension [12,21]. The stress field in the bulk together with residual surface stress can be regarded as a residual stress field in the nano structures, which are non-homogeneous and are associated with zero traction on the boundary of nano structures in general. This self equilibrium state (without external loadings) under the action of surface tension is usually chosen as the reference configuration, from which nano structures will elastically deform. Some researchers [22–25] have recognized the importance of surface tension, but often neglect the effects of the residual stress field in the bulk on the mechanical response of nano structures. Therefore, in this paper, the influences of the surface tension and the residual stress field in the bulk induced by surface tension on the elastic deformations of nano structures will be studied.

Since one-dimensional (1D) nano structures, such as nanowires and nano beams, have significant applications as nano components of electronic devices, sensors, actuators and nano electromechanical systems (NEMS) [26–28], the accurate analysis of mechanical properties of individual 1D nano structures is required in functional design and reliability analysis of those nano devices. In this paper, we will investigate the pure bending of Al nanowires to illustrate how the surface tension and the residual stress induced by the surface tension will affect the effective Young's modulus of nanowires.

The paper is organized as follows. The geometry and kinematics of a deformable surface both in the Lagrangian and in the Eulerian descriptions will be introduced in Section 2; the emphasis is placed on the study of the relations of these two descriptions at infinitesimal deformations. The isotropic surface elasticity at small deformations will be discussed in Section 3. The residual stress field in the bulk induced by surface tension will be analyzed and the corresponding constitutive relations of the bulk are formulated in Section 4. As an illustration, in Section 5, the effective Young's modulus of an Al nanowire under pure bending will be calculated. It is shown that the surface tension will affect the bending properties of nanowires.

2. Geometry and kinematics of a deformable surface

There are two kinds of methods to describe the deformation of a continuum, i.e. the Lagrangian and the Eulerian descriptions. In this section, we will adopt these two ways to describe the geometry and kinematics of a deformable surface and give the correlations of these two descriptions at infinitesimal deformations.

2.1. Geometrical relations

In the reference configuration, we consider a smooth surface A_0 in three-dimensional Euclidean space determined by the parametric representation $\mathbf{Y} = \mathbf{Y}(\theta^1, \theta^2)$, where $\mathbf{Y}$ is the position vector from the origin to points on the surface, and the parameters θ^α (the Greek indices have the range 1, 2 in this paper) serve as curvilinear coordinates on the surface. In the reference configuration, the covariant base vectors $\mathbf{A}_\alpha$ of the surface A_0 are defined as

$$\mathbf{A}_\alpha = \mathbf{Y}_{,\alpha}, \tag{1}$$

where the comma notation is used to denote partial derivatives with respect to θ^α in the present paper. The contra-variant base vectors $\mathbf{A}^\beta$ of the surface A_0 are given by

$$\mathbf{A}^\beta \cdot \mathbf{A}_\alpha = \delta^\beta_\alpha, \tag{2}$$

where δ^β_α is the Kronecker delta symbol in two dimensional space.

After deformation, the point $\mathbf{Y}$ on surface A_0 will move to the point $\mathbf{y}(\theta^1, \theta^2)$ on surface A in the current configuration. The corresponding covariant and contra-variant base vectors of surface A are

$$\mathbf{a}_\alpha = \mathbf{y}_{,\alpha} \quad \text{and } \mathbf{a}^\beta \cdot \mathbf{a}_\alpha = \delta^\beta_\alpha. \tag{3}$$

Base vectors $\mathbf{A}_\alpha$ (or $\mathbf{a}_\alpha$) span the tangent plane of the surface at $\mathbf{Y}$ (or $\mathbf{y}$) in the reference (or current) configuration. Assume that there is a linear transformation that maps a vector in the tangent plane of the undeformed surface into a vector in the tangent plane of the deformed surface (see Fig. 1). This mapping is called as the surface deformation gradient (denoted by $\mathbf{F}_s$), which is a two-point tensor and can be represented as

$$\mathbf{F}_s = \mathbf{a}_\alpha \otimes \mathbf{A}^\alpha, \tag{4}$$

where the Einstein summation convention over repeated indices is implied in the present paper. Correspondingly, we can define its inverse transformation $\mathbf{F}_s^{-1}$, so that

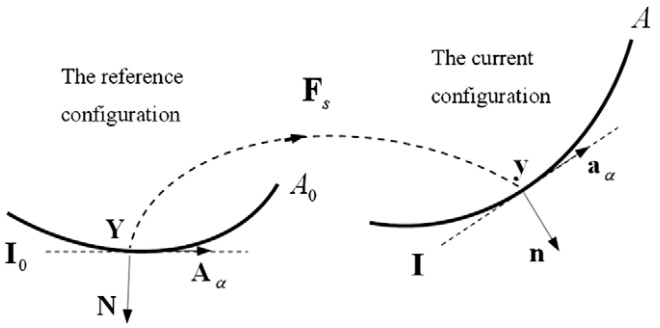

Fig. 1. The deformation of a surface.

$$\mathbf{F}_s^{-1} = \mathbf{A}_\alpha \otimes \mathbf{a}^\alpha. \tag{5}$$

It can be seen that

$$\begin{aligned} &\mathbf{F}_s \cdot \mathbf{F}_s^{-1} = \mathbf{I}, \quad \mathbf{F}_s^{-1} \cdot \mathbf{F}_s = \mathbf{I}_0, \\ &\mathbf{F}_s \cdot \mathbf{I}_0 = \mathbf{I} \cdot \mathbf{F}_s = \mathbf{F}_s, \quad \mathbf{F}_s^{-1} \cdot \mathbf{I} = \mathbf{I}_0 \cdot \mathbf{F}_s^{-1} = \mathbf{F}_s^{-1}, \end{aligned} \tag{6}$$

where $\mathbf{I}_0 = \mathbf{A}_\alpha \otimes \mathbf{A}^\alpha$ and $\mathbf{I} = \mathbf{a}_\alpha \otimes \mathbf{a}^\alpha$ are identity tensors on the tangent planes of the surface before and after deformations, respectively.

In the reference and the current configurations, we define two surface deformation tensors $\mathbf{C}_s = \mathbf{F}_s^T \cdot \mathbf{F}_s$ and $\mathbf{B}_s^{-1} = \mathbf{F}_s^{-T} \cdot \mathbf{F}_s^{-1}$. It can be proved that $\mathbf{C}_s$ and $\mathbf{B}_s^{-1}$ are positive-definite. Therefore, we can introduce two tensors

$$\mathbf{U}_s = \sqrt{\mathbf{C}_s}, \quad \mathbf{V}_s^{-1} = \sqrt{\mathbf{B}_s^{-1}}. \tag{7}$$

Then, the following decompositions hold

$$\mathbf{F}_s = \mathbf{R}_s \cdot \mathbf{U}_s = \mathbf{V}_s \cdot \mathbf{R}_s, \tag{8}$$

where $\mathbf{R}_s$ is the two-point rotation tensor satisfying

$$\begin{aligned} &\mathbf{R}_S^T \cdot \mathbf{R}_S = \mathbf{I}_0, \quad \mathbf{R}_s \cdot \mathbf{R}_S^T = \mathbf{I}, \\ &\mathbf{R}_S \cdot \mathbf{I}_0 = \mathbf{R}_S, \quad \mathbf{I} \cdot \mathbf{R}_s = \mathbf{R}_s. \end{aligned} \tag{9}$$

From (1) to (3), the displacement vector $\mathbf{u}$ of a point on the surface either in the reference configuration or in the current configuration can be written as

$$\mathbf{u} = \mathbf{y} - \mathbf{Y} = u_0^\alpha \mathbf{A}_\alpha + u_0^n \mathbf{N} = u^\alpha \mathbf{a}_\alpha + u^n \mathbf{n} \tag{10}$$

in which $\mathbf{N}$ and $\mathbf{n}$ are unit normal vectors of the surface before and after deformations, respectively. From (1), (3) and (10), we have the following relations between $\mathbf{A}_\alpha$ and $\mathbf{a}_\alpha$

$$\begin{aligned} \mathbf{a}_\alpha &= \mathbf{A}_\alpha + \left[\left(u_0^\lambda|_\alpha - u_0^n b_{0\alpha}^\lambda\right)\mathbf{A}_\lambda + \left(u_0^\beta b_{0\alpha\beta} + u_{0,\alpha}^n\right)\mathbf{N}\right], \\ \mathbf{A}_\alpha &= \mathbf{a}_\alpha - \left[\left(u^\lambda\|_\alpha - u^n b_\alpha^\lambda\right)\mathbf{a}_\lambda + \left(u^\beta b_{\alpha\beta} + u_{,\alpha}^n\right)\mathbf{n}\right], \end{aligned} \tag{11}$$

where $u_0^\lambda|_\alpha$ and $u^\lambda\|_\alpha$ are defined by

$$\begin{aligned} u_0^\lambda|_\alpha &= u_{0,\alpha}^\lambda + u_0^\beta \overline{\Gamma}_{0\alpha\beta}^\lambda, \\ u^\lambda\|_\alpha &= u_{,\alpha}^\lambda + u^\beta \overline{\Gamma}_{\alpha\beta}^\lambda; \end{aligned} \tag{12}$$

$\overline{\Gamma}_{0\alpha\beta}^\lambda$ and $\overline{\Gamma}_{\alpha\beta}^\lambda$ are the Christoffel symbols of the second kind of the surface before and after deformations; and the surface curvature tensors in the reference and the current configurations can be expressed as

$$\begin{aligned} \mathbf{b}_0 &= b_{0\alpha}^\lambda \mathbf{A}_\lambda \otimes \mathbf{A}^\alpha = b_{0\alpha\beta}\mathbf{A}^\alpha \otimes \mathbf{A}^\beta, \\ \mathbf{b} &= b_\alpha^\lambda \mathbf{a}_\lambda \otimes \mathbf{a}^\alpha = b_{\alpha\beta}\mathbf{a}^\alpha \otimes \mathbf{a}^\beta. \end{aligned} \tag{13}$$

From Eq. (11), $\mathbf{F}_s$ and $\mathbf{F}_s^{-1}$ can be written as

$$\begin{aligned} \mathbf{F}_s &= \mathbf{I}_0 + \mathbf{u}_0 \overline{\nabla}_{0s} + \mathbf{F}_s^{(o)}, \\ \mathbf{F}_s^{-1} &= \mathbf{I} - \left[\mathbf{u}\overline{\nabla}_s + \widetilde{\mathbf{F}}_s^{(o)}\right], \end{aligned} \tag{14}$$

where

$$\mathbf{u}_0\bar{\nabla}_{0s} = \left(u_0^{\lambda}\big|_{\alpha} - u_0^n b_0 \alpha^{\lambda}\right)\mathbf{A}_{\lambda}\otimes\mathbf{A}^{\alpha}, \quad \mathbf{F}_s^{(o)} = \left(u_0^{\beta}b_{0\alpha\beta} + u_{0,\alpha}^n\right)\mathbf{N}\otimes\mathbf{A}^{\alpha}, \tag{15}$$

$$\mathbf{u}\bar{\nabla}_s = \left(u^{\lambda}\|_{\alpha} - u^n b_{\alpha}^{\lambda}\right)\mathbf{a}_{\lambda}\otimes\mathbf{a}^{\alpha}, \quad \widetilde{\mathbf{F}}_s^{(o)} = \left(u^{\beta}b_{\alpha\beta} + u_{,\alpha}^n\right)\mathbf{n}\otimes\mathbf{a}^{\alpha}. \tag{16}$$

$\mathbf{F}_s^{(o)}$ denotes the out-plane term of $\mathbf{F}_s$ in the reference configuration; $\widetilde{\mathbf{F}}_s^{(o)}$ is the corresponding out-plane term of $\mathbf{F}_s^{-1}$ in the current configuration. Therefore, we have

$$\begin{aligned}\mathbf{C}_s &= \mathbf{I}_0 + \bar{\nabla}_{0s}\mathbf{u}_0 + \mathbf{u}_0\bar{\nabla}_{0s} + \bar{\nabla}_{0s}\mathbf{u}_0\cdot\mathbf{u}_0\bar{\nabla}_{0s} + \mathbf{F}_s^{T(o)}\cdot\mathbf{F}_s^{(o)},\\ \mathbf{B}_s^{-1} &= \mathbf{I} - \bar{\nabla}_s\mathbf{u} - \mathbf{u}\bar{\nabla}_s + \bar{\nabla}_s\mathbf{u}\cdot\mathbf{u}\bar{\nabla}_s + \widetilde{\mathbf{F}}_s^{T(o)}\cdot\widetilde{\mathbf{F}}_s^{(o)}.\end{aligned} \tag{17}$$

2.2. Surface velocity gradient and rate of deformation

Velocity vector of a point $\mathbf{y}$ on the deformed surface A is $\mathbf{v}_s = \frac{\partial\mathbf{y}}{\partial t}$. Its gradient can be expressed by the material derivative of $\mathbf{F}_s$ as

$$\mathbf{L}_s = \mathbf{v}_{s,\alpha}\otimes\mathbf{a}^{\alpha} = \frac{\partial(\mathbf{y}_{,\alpha})}{\partial t}\otimes\mathbf{a}^{\alpha} = \dot{\mathbf{a}}_{\alpha}\otimes\mathbf{a}^{\alpha} = (\dot{\mathbf{a}}_{\alpha}\otimes\mathbf{A}^{\alpha})\cdot(\mathbf{A}_{\beta}\otimes\mathbf{a}^{\beta}) = \dot{\mathbf{F}}_s\cdot\mathbf{F}_s^{-1} \tag{18}$$

and the symmetrical part of $\mathbf{L}_s$ is

$$\widetilde{\mathbf{D}}_s = \frac{1}{2}\left(\mathbf{L}_s + \mathbf{L}_s^T\right) = \frac{1}{2}\left(\dot{\mathbf{F}}_s\cdot\mathbf{F}_s^{-1} + \mathbf{F}_s^{-T}\cdot\dot{\mathbf{F}}_s^T\right). \tag{19}$$

Since $\widetilde{\mathbf{D}}_s$ has out-plane terms in the current configuration, we define the rate of deformation of the surface as follows:

$$\mathbf{D}_s = \mathbf{I}\cdot\widetilde{\mathbf{D}}_s\cdot\mathbf{I} = \frac{1}{2}\left(\mathbf{I}\cdot\dot{\mathbf{F}}_s\cdot\mathbf{F}_s^{-1} + \mathbf{F}_s^{-T}\cdot\dot{\mathbf{F}}_s^T\cdot\mathbf{I}\right). \tag{20}$$

It can be seen that

$$\mathbf{D}_s = \frac{1}{2}\mathbf{F}_s^{-T}\cdot\dot{\mathbf{C}}_s\cdot\mathbf{F}_s^{-1}, \tag{21}$$

where

$$\dot{\mathbf{C}}_s = \left(\dot{\mathbf{F}}_s^T\cdot\mathbf{F}_s + \mathbf{F}_s^T\cdot\dot{\mathbf{F}}_s\right), \tag{22}$$

which yields

$$\dot{\mathbf{C}}_s = 2\mathbf{F}_s^T\cdot\mathbf{D}_s\cdot\mathbf{F}_s. \tag{23}$$

The relations between $\dot{\mathbf{C}}_s$ and $\mathbf{D}_s$ are similar to those of three-dimensional continuum mechanics.

2.3. Infinitesimal deformation approximations

The surface deformation tensors $\mathbf{C}_s$ and $\mathbf{B}_s^{-1}$ and their material derivatives are nonlinear in the displacement gradient and, consequently, in the displacements. However, it is reasonable and convenient to use the linearized expressions under infinitesimal deformations. Thus, the high-order small quantities of the surface displacement gradient will be neglected in the following analyses. Therefore, we have

$$\mathbf{C}_s = \mathbf{I}_0 + 2\mathbf{E}_s, \quad \mathbf{B}_s^{-1} = \mathbf{I} - 2\boldsymbol{\varepsilon}_s \tag{24}$$

in which

$$\mathbf{E}_s = \frac{1}{2}\left(\bar{\nabla}_{0s}\mathbf{u}_0 + \mathbf{u}_0\bar{\nabla}_{0s}\right), \boldsymbol{\varepsilon}_s = \frac{1}{2}\left(\bar{\nabla}_s\mathbf{u} + \mathbf{u}\bar{\nabla}_s\right). \tag{25}$$

Consequently, $\mathbf{F}_s^{-1}$ can be expressed in the reference configuration as

$$\mathbf{F}_s^{-1} = \mathbf{C}_s^{-1}\cdot\mathbf{F}_s^T = (\mathbf{I}_0 - 2\mathbf{E}_s)\left(\mathbf{I}_0 + \bar{\nabla}_{0s}\mathbf{u}_0 + \mathbf{F}_s^{(o)T}\right) = \mathbf{I}_0 - \mathbf{u}_0\bar{\nabla}_{0s} + \mathbf{F}_s^{(o)T}. \tag{26}$$

Hence, the identity tensor $\mathbf{I}$ in the tangent plane of the current configuration can be given by

$$\mathbf{I} = \mathbf{F}_s\cdot\mathbf{F}_s^{-1} = \mathbf{I}_0 + \left(\mathbf{F}_s^{(o)T} + \mathbf{F}_s^{(o)}\right). \tag{27}$$

It is shown that, even in the case of infinitesimal deformation, the identity tensors in different configurations are not the same. The differences are the out-plane terms of surface deformation gradient. That is to say, the current identity tensor $\mathbf{I}$ is dependent on the deformation even in the case of small deformations.

Substituting Eq. (26) into the expression of $\mathbf{B}_s^{-1}$, we obtain

$$\mathbf{B}_s^{-1} = \mathbf{F}_s^{-T} \cdot \mathbf{F}_s^{-1} = \mathbf{I}_0 - 2\mathbf{E}_s + \left(\mathbf{F}_s^{(o)T} + \mathbf{F}_s^{(o)}\right). \tag{28}$$

From (24), (27) and (28), it follows that:

$$\mathbf{E}_s = \boldsymbol{\varepsilon}_s. \tag{29}$$

This means that although the identity tensors in different configurations are not the same, the surface strain tensors are equal in infinitesimal deformation approximation.

Under infinitesimal deformations, Eq. (19) becomes

$$\widetilde{\mathbf{D}}_s = \dot{\mathbf{E}}_s + \frac{1}{2}\left(\dot{\mathbf{F}}_s^{(o)} + \dot{\mathbf{F}}_s^{(o)T}\right), \tag{30}$$

where

$$\dot{\mathbf{E}}_s = \frac{1}{2}\dot{\mathbf{C}}_s = \frac{1}{2}\left(\dot{\mathbf{u}}_0 \bar{\nabla}_{0s} + \bar{\nabla}_{0s}\dot{\mathbf{u}}_0\right). \tag{31}$$

Accordingly, we have

$$\mathbf{D}_s = \dot{\mathbf{E}}_s. \tag{32}$$

This indicates that the strain rate tensors are the same under small deformations.

3. Surface elasticity under infinitesimal deformations

The surface Cauchy stress $\boldsymbol{\sigma}_s$ measures the force per unit length in the deformed surface. In many problems of interest, it is not convenient to work with $\boldsymbol{\sigma}_s$, since the deformed configuration is not known in advance. For this reason, we introduce other two surface stress tensors, namely the first and the second surface Piola-Kirchhoff stress tensors, $\mathbf{S}_s$ and $\mathbf{T}_s$, which give the force measured per unit length in the reference configuration. These stress tensors should satisfy the following work conjugate relations:

$$\dot{w}_s = J_2 \boldsymbol{\sigma}_s : \mathbf{D}_s = \mathbf{S}_s : \dot{\mathbf{F}}_s = \frac{1}{2}\mathbf{T}_s : \dot{\mathbf{C}}_s, \tag{33}$$

where $w_s = J_2\gamma$ is the surface energy per unit area of surface A_0 in the reference configuration, and $J_2 = \det\mathbf{U}_s$ is the ratio between the area elements of after and before deformations. The proofs of Eq. (33) are given in the Appendix A.

For hyperelastic media, the surface energy density γ can be assumed to be a function of $\mathbf{U}_s$(or $\mathbf{C}_s$). In particular, for an isotropic surface, γ can be written as a function of the first and second invariants of $\mathbf{U}_s$, namely J_1 (or $\mathrm{tr}\mathbf{U}_s$) and J_2. Hence, under the Lagrangian description, the surface constitutive relation can be written as in Refs. [12,13]:

$$\mathbf{T}_s = 2\frac{\partial(J_2\gamma)}{\partial \mathbf{C}_s}, \tag{34}$$

which is related to the first surface Piola-Kirchhoff stress tensors $\mathbf{S}_s$ and surface Cauchy stress $\boldsymbol{\sigma}_s$ through the following relations:

$$\mathbf{S}_s = \mathbf{F}_s \cdot \mathbf{T}_s, \quad \boldsymbol{\sigma}_s = \frac{1}{J_2}\mathbf{F}_s \cdot \mathbf{T}_s \cdot \mathbf{F}_s^T.$$

In the case of small deformations, J_1 and J_2 can be approximately expressed by

$$J_1 = 2 + \mathrm{tr}\mathbf{E}_s, \quad J_2 = 1 + \mathrm{tr}\mathbf{E}_s + \det\mathbf{E}_s. \tag{35}$$

Correspondingly, γ can be expressed as a series expansion [13,29]

$$\gamma = \gamma_0 + \gamma_1(J_1 - 2) + \gamma_2(J_2 - 1) + \frac{1}{2}\gamma_{11}(J_1 - 2)^2 + \gamma_{12}(J_1 - 2)(J_2 - 1) + \frac{1}{2}\gamma_{22}(J_2 - 1)^2 + \ldots \tag{36}$$

Hence, by using Eqs. (34)–(36) and neglecting high-order small quantities, we have

$$\mathbf{T}_s = \gamma_0^*\mathbf{I}_0 + (\gamma_0^* + \gamma_1^*)(\mathrm{tr}\mathbf{E}_s)\mathbf{I}_0 + (\gamma_1 - 2\gamma_0^*)\mathbf{E}_s, \tag{37}$$

where $\gamma_0^* = \gamma_0 + \gamma_1 + \gamma_2$, $\gamma_1^* = \gamma_1 + 2\gamma_2 + \gamma_{11} + 2\gamma_{12} + \gamma_{22}$. The surface energy γ_0, residual surface stress (namely surface tension) γ_0^* and surface elastic constants γ_1^* and γ_1 are material properties intrinsic to the solid [11,15]. The condition of thermodynamic stability requires that surface energy γ_0 should be positive. However, the residual surface stress γ_0^* and surface elastic constants γ_1^* and γ_1 may be either positive or negative depending on the atomic or molecular arrangement on the surface [15].

In the Lagrangian description, the first kind of surface Piola-Kirchhoff stress can be expressed by [13]

$$\mathbf{S}_s = \gamma_0^*\mathbf{I}_0 + \left(\gamma_0^* + \gamma_1^*\right)(\mathrm{tr}\mathbf{E}_s)\mathbf{I}_0 - \gamma_0^*(\bar{\nabla}_{0s}\mathbf{u}_0) + \gamma_1\mathbf{E}_s + \gamma_0^*\mathbf{F}_s^{(o)} \tag{38}$$

in which the last term is related to the out-plane term of the surface deformation gradient.

In the Eulerian description, stress–strain relation of the surface can be written as

$$\boldsymbol{\sigma}_s = \gamma_0^*\mathbf{I} + \gamma_1^*(\mathrm{tr}\boldsymbol{\varepsilon}_s)\mathbf{I} + \gamma_1\boldsymbol{\varepsilon}_s. \tag{39}$$

By using Eqs. (27) and (29), the above model can also be expressed, in the undeformed configuration, as

$$\boldsymbol{\sigma}_s = \gamma_0^*\mathbf{I}_0 + \gamma_1^*(\mathrm{tr}\mathbf{E}_s)\mathbf{I}_0 + \gamma_1\mathbf{E}_s + \gamma_0^*\left(\mathbf{F}_s^{(o)} + \mathbf{F}_s^{(o)T}\right). \tag{40}$$

This means that there are out-plane terms when surface Cauchy stress is expressed under the frame of the reference configuration. Thus, even in the case of small deformations, it is needed to discriminate the reference and the current configurations of the surface. Some researchers pay no attention to the difference between (39) and (40), and often neglect the out-plane terms, which are important for curved and rotated surfaces. It can be seen that, even in the case of infinitesimal deformations, different surface stress tensors in Eqs. (37)–(40) are not the same due to the existence of the residual stress γ_0^*.

4. Elasticity for the bulk with residual stress fields

Atoms at or near a free surface experience reduced coordination due to a different local binding environment than the interior atoms. As a consequence of under-coordination, the surface will be subjected to a residual stress, namely surface tension. In order to keep equilibrium, a residual stress field in the bulk will be induced by surface tension in the reference configuration that is not subjected to any external loading.

4.1. Determination of the residual stress in the bulk

For nano scale structures, according to the generalized Young-Laplace equations which describes the equilibrium conditions of the surface (details can be found in Appendix B), the presence of surface tension will result in a non-classical boundary condition which gives the traction on the bulk in terms of surface tension. This boundary condition together with the equations of classical elasticity (to be satisfied within the bulk) forms a coupled system of field equations to determine the residual stress in the bulk [12,21].

In the reference configurations, from Eq. (B2) and noting that $\boldsymbol{\sigma}_s = \gamma_0^*\mathbf{I}_0$ for isotropic materials, the elastic stress field $\widehat{\mathbf{T}}$ in the bulk should satisfy [12]

$$\widehat{\mathbf{T}}\cdot\nabla = 0 \quad \text{(in the bulk)} \tag{41}$$

$$\mathbf{N}\cdot[\![\widehat{\mathbf{T}}]\!]\cdot\mathbf{N} = -\gamma_0^*\mathbf{I}_0 : \mathbf{b}_0, \quad \text{(on the surface)} \tag{42}$$

$$\mathbf{P}_0\cdot[\![\widehat{\mathbf{T}}]\!]\cdot\mathbf{N} = -\nabla_{0s}\gamma_0^*,$$

where $\mathbf{P_0} = \mathbf{1} - \mathbf{N}\otimes\mathbf{N}$ is the perpendicular projection of the space of all vectors upon the space of tangential vectors in the reference configuration, $\mathbf{1}$ is the identity tensor on 3-dimentional Euclidean space.

Based on the above equations, a large deformation analysis for the determination of the residual stress in an infinite medium containing a spherical nano-cavity was given in [12]

4.2. Elasticity with residual stress

The elastic field which is induced by the surface tension is referred to as the residual elastic field. Thus, the bulk of nano structure materials will deform elastically from a residual stressed state. It should be pointed out that, in the prediction of mechanical properties of nano structures, the classical Hooke's law is often used to describe the elastic response of the bulk, where the residual stress is neglected. This may not be reasonable. It is because the constitutive relations of linear elastic materials with residual stress are quite different from the classical Hooke's law [30].

In view of the importance of the linearization of the general constitutive equations, we will present the linear elastic constitutive relations of the bulk with residual stresses as follows [30]:

$$\mathbf{S} = \widehat{\mathbf{T}} + \mathbf{H}\cdot\widehat{\mathbf{T}} - \frac{1}{2}(\mathbf{E}\cdot\widehat{\mathbf{T}} + \widehat{\mathbf{T}}\cdot\mathbf{E}) + \lambda(\mathrm{tr}\mathbf{E})\mathbf{1} + 2\mu\mathbf{E}, \tag{43}$$

where $\mathbf{S}$ is the first Piola-Kirchhoff stress, $\widehat{\mathbf{T}}$ is the residual stress in the reference configuration, $\mathbf{H}$ is the displacement gradient calculated from the reference configuration, $\mathbf{E}$ is the infinitesimal strain, λ and μ are material elastic constants.

Accordingly, the Cauchy stress can be written as [30]

$$\boldsymbol{\sigma} = \widehat{\mathbf{T}} + \mathbf{W}\cdot\widehat{\mathbf{T}} - \widehat{\mathbf{T}}\cdot\mathbf{W} + \frac{1}{2}(\mathbf{E}\cdot\widehat{\mathbf{T}} + \widehat{\mathbf{T}}\cdot\mathbf{E}) - (\mathrm{tr}\mathbf{E})\widehat{\mathbf{T}} + \lambda\mathrm{tr}(\mathbf{E})\mathbf{1} + 2\mu\mathbf{E} \tag{44}$$

in which $\mathbf{W} = \frac{1}{2}(\mathbf{H} - \mathbf{H}^T)$ is the infinitesimal rotation tensor.

5. Pure bending of nanowires

Due to the distinct mechanical properties of structures at nano scale, nanowires have attracted considerable interests. Both atom simulations [31,32] and theoretical studies [15,23,24,33,34] have shown that free surfaces will affect the elastic modulus or stiffness of nanowires, which control their capacities for deformation during sensing and actuation. In most previous works, theoretical analyses were based on the Eulerian surface elasticity, in which the out-plane terms of surface stress were neglected and the effect of residual stress in the bulk was not taken into account. As an illustration, in this section, we will consider the effects of these factors on pure bending of a nanowire, which are not considered by previous authors. The wire is assumed to be isotropic and under linear elastic responses. The coordinate system with origin at the middle of the line, which lies both in the neutral surface and in the cross section of the middle of the wire, is shown in Fig. 2. The x-axis is parallel to the axis of the unbent wire and the y- and z-axes are perpendicular to it. l, h and b are the length, thickness and width of the wire in the reference configuration, respectively.

For the nanowires with rectangle cross section (as shown in Fig. 3a), the cross section can be described by a rounded rectangle, of which the radius is r (see Fig. 3b). Consider a quarter of the cylinder of the bulk material at the corner (as shown Fig. 3c). From the generalized Young-Laplace equations (42), the existence of surface tension γ_0^* on the cylindrical surface leads to a pressure (or traction) p acting on corresponding boundary of the bulk material (see Fig. 3c), which has magnitude γ_0^*/r. The equilibrium conditions require the forces F_y and F_z acting on the lateral sides of the element (as shown Fig. 3c). It can be solved that F_y and F_z are equal in magnitude and have the values γ_0^*, which is independent of the radius r. When r approaches zero, the rounded rectangle cross section is close to the real case. Therefore, the corner of the bulk material at point A will be under the actions F_y and F_z, which has been shown in Fig. 3a. The forces acting on other corners can be obtained through the same methods. Using a finite element analysis, Gurtin and Murdoch [21] solved the residual stress in the bulk, which is a non-homogeneous stress field. In order to consider the effects of residual stress in the bulk on the apparent Young's modulus of nanowires, we will simplify the non-homogenous residual stress field in the bulk under the equivalence principle. We assume that the non-homogenous distributed range of the residual stress is small, which closely near the corners, and that the stress at the points away from the corners is uniformly distributed. Hence, from the equilibrium conditions of the bulk material, we can get the stress acting on the plane $A'A'$ is $\widehat{T}_{yy} = -2\gamma_0^*/h$, which is uniformly distributed along the thickness and is inversely proportional to the thickness of the nanowires. Similarly, the residual stresses along other directions in the bulk can be acquired. Here, the components of the residual stress in the bulk are

$$\widehat{T}_{ij} = \mathbf{e}_i \cdot \widehat{\mathbf{T}} \cdot \mathbf{e}_j = \begin{pmatrix} -2\gamma_0^*\left(\frac{1}{b}+\frac{1}{h}\right) & 0 & 0 \\ 0 & -\frac{2\gamma_0^*}{h} & 0 \\ 0 & 0 & -\frac{2\gamma_0^*}{b} \end{pmatrix}, \tag{45}$$

where $i, j = x, y, z$; $\mathbf{e}_i$ are the unit orthonormal vectors.

We further assume that plane sections remain plane during the bending process and the Poisson's ratio of the surface is equal to that of the bulk. According to the elastic theory [35], the displacements for pure bending of a nanowire can be described as

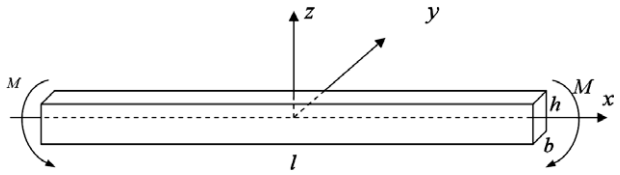

Fig. 2. Pure bending of a nanowire.

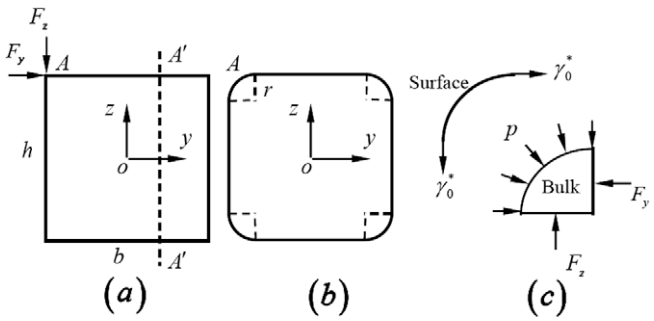

Fig. 3. Nanowire with rectangle cross section.

$$u_x = \frac{xz}{R},$$
$$u_y = -v\frac{yz}{R}, \tag{46}$$
$$u_z = -\frac{1}{2R}[x^2 + v(z^2 - y^2)],$$

where v is the Poisson's ratio, R is the curvature radius of the neutral surface after bending.

Hence, the components of displacements gradient $\mathbf{H}$ for the bulk material are

$$H_{ij} = \mathbf{e}_i \cdot \mathbf{H} \cdot \mathbf{e}_j = \begin{pmatrix} \frac{z}{R} & 0 & \frac{x}{R} \\ 0 & -v\frac{z}{R} & -v\frac{y}{R} \\ -\frac{x}{R} & v\frac{y}{R} & -v\frac{z}{R} \end{pmatrix}, \tag{47}$$

and the infinitesimal strain is given by

$$E_{ij} = \mathbf{e}_i \cdot \left(\frac{\mathbf{H} + \mathbf{H}^T}{2}\right) \cdot \mathbf{e}_j = \begin{pmatrix} \frac{z}{R} & 0 & 0 \\ 0 & -v\frac{z}{R} & 0 \\ 0 & 0 & -v\frac{z}{R} \end{pmatrix}. \tag{48}$$

Substituting (45), (47) and (48) into (43), we obtain the stress components for the bulk material

$$S_{ij} = \mathbf{e}_i \cdot \mathbf{S} \cdot \mathbf{e}_j = \begin{pmatrix} \widehat{T}_{11} + E\frac{z}{R} & 0 & \widehat{T}_{33}\frac{x}{R} \\ 0 & \widehat{T}_{22} & -\widehat{T}_{33}\frac{vy}{R} \\ -\widehat{T}_{11}\frac{x}{R} & \widehat{T}_{22}\frac{vy}{R} & \widehat{T}_{33} \end{pmatrix}, \tag{49}$$

where E is bulk Young's modulus.

For the upper and the lower surfaces $(x, y, \pm\frac{h}{2})$, the components of surface displacement gradient $\mathbf{H}^s = \mathbf{F}_s - \mathbf{I}_0$ are

$$H^s_{i\alpha} = \mathbf{e}_i \cdot \mathbf{H}^s \cdot \mathbf{e}_\alpha = \begin{pmatrix} \frac{1}{R}\left(\pm\frac{h}{2}\right) & 0 \\ 0 & -\frac{v}{R}\left(\pm\frac{h}{2}\right) \\ -\frac{x}{R} & v\frac{y}{R} \end{pmatrix}, \tag{50}$$

where $\alpha = x, y$, the sign "±" is "+" for upper surface and "−" for lower surface. Thus, the surface strain components are

$$E^s_{\alpha\beta} = \mathbf{e}_\alpha \cdot \left(\frac{\mathbf{H}^s + \mathbf{H}^{sT}}{2}\right) \cdot \mathbf{e}_\beta = \begin{pmatrix} \frac{1}{R}\left(\pm\frac{h}{2}\right) & 0 \\ 0 & -\frac{v}{R}\left(\pm\frac{h}{2}\right) \end{pmatrix}. \tag{51}$$

Substituting (50) and (51) into (38), we obtain the surface stress components for the upper and lower surfaces

$$S^s_{i\alpha} = \mathbf{e}_i \cdot \mathbf{S}^s \cdot \mathbf{e}_\alpha = \begin{pmatrix} \gamma_0^* + E_s\frac{1}{R}\left(\pm\frac{h}{2}\right) & 0 \\ 0 & \gamma_0^* \\ -\gamma_0^*\frac{x}{R} & \gamma_0^* v\frac{y}{R} \end{pmatrix}, \tag{52}$$

where the definitions of the surface Poisson's ratio $v\left(v = \frac{\gamma_0^* + \gamma_1^*}{\gamma_1^* + \gamma_1}\right)$ and the surface Young's modulus $E_s\left(E_s = \gamma_1^* + \gamma_1 - \frac{(\gamma_0^* + \gamma_1^*)^2}{\gamma_1^* + \gamma_1}\right)$ are used to simplify S^s_{xx} and S^s_{yy}.

For the anterior and the posterior surfaces $(x, \pm\frac{b}{2}, z)$, the components of surface displacement gradient are

$$H^s_{i\alpha} = \mathbf{e}_i \cdot \mathbf{H}^s \cdot \mathbf{e}_\alpha = \begin{pmatrix} \frac{z}{R} & \frac{x}{R} \\ 0 & -\frac{v}{R}\left(\pm\frac{b}{2}\right) \\ -\frac{x}{R} & -v\frac{z}{R} \end{pmatrix}, \tag{53}$$

where $\alpha = x, z$, and the sign "±" is "+" for anterior surface and "−" for posterior surface. Hence, we have

$$E^s_{\alpha\beta} = \mathbf{e}_\alpha \cdot \left(\frac{\mathbf{H}^s + \mathbf{H}^{sT}}{2}\right) \cdot \mathbf{e}_\beta = \begin{pmatrix} \frac{z}{R} & 0 \\ 0 & -v\frac{z}{R} \end{pmatrix}. \tag{54}$$

Substituting (53) and (54) into (38), we obtain

$$S^s_{i\alpha} = \mathbf{e}_i \cdot \mathbf{S}^s \cdot \mathbf{e}_\alpha = \begin{pmatrix} \gamma_0^* + E_s\frac{z}{R} & \gamma_0^*\frac{x}{R} \\ 0 & -\gamma_0^*\frac{v}{R}\left(\pm\frac{b}{2}\right) \\ -\gamma_0^*\frac{x}{R} & \gamma_0^* \end{pmatrix}. \tag{55}$$

Next, we adopt the principle of virtual work to get the effective modulus of nanowires. Consider an arbitrary geometrically permissible displacement fields $\left(\dot{H}_{ij}, \dot{H}^s_{i\alpha}\right)$ for pure bending. The corresponding principle of virtual work becomes

$$M \cdot \dot{\kappa} l = \dot{W}_B + \dot{W}^{UL}_S + \dot{W}^{AP}_S, \tag{56}$$

where M is the bending moment, $\dot{\kappa}$ is the curvature change of the neutral surface; and $\dot{W}_B$, $\dot{W}^{UL}_S$ and $\dot{W}^{AP}_S$ are the virtual strain energy of the bulk, of the upper and the lower surfaces and of the anterior and the posterior surfaces, respectively. From Eqs. (47)–(55), we have

$$\begin{aligned}
\dot{W}_B &= \int_{-\frac{l}{2}}^{\frac{l}{2}} \int_{-\frac{b}{2}}^{\frac{b}{2}} \int_{-\frac{h}{2}}^{\frac{h}{2}} S_{ij}\dot{H}_{ij} dz dy dx = l\dot{\kappa}\frac{I}{R}\left[E + (\widehat{T}_{11} + \widehat{T}_{33})\left(\frac{l}{h}\right)^2 + (\widehat{T}_{22} + \widehat{T}_{33})\nu^2\left(\frac{b}{h}\right)^2\right], \\
\dot{W}^{UL}_S &= \int_{-\frac{l}{2}}^{\frac{l}{2}} \int_{-\frac{b}{2}}^{\frac{b}{2}} S^s_{i\alpha}\dot{H}^s_{i\alpha} dy dx = l\dot{\kappa}\frac{I}{R}\left[6\frac{E_s}{h} + 2\frac{\gamma^*_0}{h}\left(\frac{l}{h}\right)^2 + 2\frac{\gamma^*_0}{h}\nu^2\left(\frac{b}{h}\right)^2\right], \\
\dot{W}^{AP}_S &= \int_{-\frac{l}{2}}^{\frac{l}{2}} \int_{-\frac{h}{2}}^{\frac{h}{2}} S^s_{i\alpha}\dot{H}^s_{i\alpha} dz dx = l\dot{\kappa}\frac{I}{R}\left[2\frac{E_s}{b} + 2\frac{\gamma^*_0}{b}\left(\frac{l}{h}\right)^2 + 6\frac{\gamma^*_0}{b}\nu^2\left(\frac{b}{h}\right)^2\right],
\end{aligned} \tag{57}$$

where $I = \frac{bh^3}{12}$.

From (45), (56) and (57), we obtain

$$M = \frac{I}{R}E', \tag{58}$$

where E' is the effective Young's modulus and can be expressed as

$$E' = E + 6\frac{E_s}{h} + 2\frac{E_s}{b} + 2\frac{\gamma^*_0}{b}\left(2\nu^2\frac{b^2}{h^2} - \frac{l^2}{h^2}\right). \tag{59}$$

It can be seen that E' is dependent on surface parameters and the geometry of the nanowires. Cuenot et al. [22] and Park and Klein [36] pointed out that the effective Young's modulus of real nanowires is strongly dependent on the boundary conditions and the geometry of the nanowires if the surface stress effects are considered. Park and Klein's numerical simulation results [36] show that, for the single crystal gold nanowires with the fixed/free boundary condition, either decreasing the thickness of nanowires or increasing the aspect ratio will lead to a decrease in the effective Young's moduli of nanowires relative to the bulk value, while increasing in the effective Young's moduli for the fixed/fixed cases. This is because that the fixed/fixed boundary conditions prevent the nanowires from relaxing axially, as would occur due to surface stresses if one of the ends were free. We theoretically investigate the pure bending properties of nanowires, which can relax axially as the fixed/free cases. When the surface tension is positive, Eq. (59) implies that the effective Young's modulus will decrease with increasing the aspect ratio. The variational trends of the effective Young's modulus are the same as those of the fixed/free nanowires obtained by Park and Klein [36].

For nanowires with square sections ($l \gg h$, $h = b$), we have

$$E' \approx E + 8\frac{E_s}{h} + 2\frac{\gamma^*_0}{h}\left(2\nu^2 - \frac{l^2}{h^2}\right). \tag{60}$$

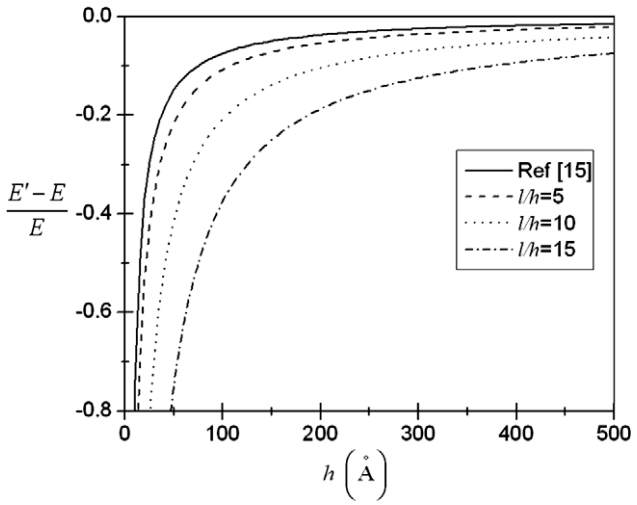

Fig. 4. Non-dimensional difference between effective Young's moduli of Al nanowires with different aspect ratio.

Note that it can be reduced to Miller and Shenoy's expression [15] by neglecting the effects of surface tension γ_0^*. $(E' - E)/E$ as a function of h for different aspect ratios of Al nanowires as shown in Fig. 4. The parameters $E_s/E = -0.9298$ Å, $\gamma_0^*/E = 0.06675$ Å, $v = 0.3$ are employed form reference [15]. Results show that surface stresses will considerably affect the effective Young's modulus of Al nanowires, which decrease with either the decrease of nanowires thickness or the increase of the aspect ratio. The trends of decreasing nanowire Young's modulus are the same as those of the fixed/free Au nanowires obtained by Park and Klein [36].

Eq. (59) is also valid for nano plates ($b \gg h$). In this case, the effective Young's modulus becomes

$$E' \approx E + 6\frac{E_s}{h} + 2\frac{\gamma_0^*}{b}\left(2v^2\frac{b^2}{h^2} - \frac{l^2}{h^2}\right), \tag{61}$$

which can also be considered as a modification of Miller and Shenoy's result [15].

6. Conclusions

This paper investigates the effects of surface tension and the residual stress field in the bulk induced by surface tension on mechanical properties of nano structures. Furthermore, the theoretical derivations about surface elasticity show that, in small deformations, equating the reference and the current configurations will make the out-plane terms of surface displacement gradient be overlooked in the Eulerian description of surface elasticity. Illustrative results of pure bending analysis of nanowires indicate that, besides surface elasticity, the surface tension will considerably affect mechanical properties of nano scale structures.

Acknowledgements

This research was jointly supported by the National Basic Research Program of China (973 Program, Grant No. 2007CB310500), the National High-tech R& D Program of China (863 Program, Grant No. 2007AA04Z348), the National Natural Science Foundation of China (NSFC, Grant No. 10772180) and the Postdoctoral Science Foundation of China (Grant No. 20080440530). These financial supports are gratefully acknowledged.

Appendix A. Work conjugate relations

Under the base vectors of the reference configuration, $\mathbf{T}_s$, $\mathbf{F}_s$ and $\dot{\mathbf{F}}_s$ can be expressed as

$$\begin{aligned}
\mathbf{T}_s &= T_\beta^\alpha \mathbf{A}_\alpha \otimes \mathbf{A}^\beta, \\
\mathbf{F}_s &= F_\eta^\gamma \mathbf{A}_\gamma \otimes \mathbf{A}^\eta + F_\eta^3 \mathbf{N} \otimes \mathbf{A}^\eta, \\
\dot{\mathbf{F}}_s &= \dot{F}_\mu^\lambda \mathbf{A}_\lambda \otimes \mathbf{A}^\mu + \dot{F}_\mu^3 \mathbf{N} \otimes \mathbf{A}^\mu.
\end{aligned} \tag{A1}$$

The relations between different surface stress tensors are

$$\mathbf{S}_s = \mathbf{F}_s \cdot \mathbf{T}_s, \quad J_2 \boldsymbol{\sigma}_s = \mathbf{F}_s \cdot \mathbf{T}_s \cdot \mathbf{F}_s^T. \tag{A2}$$

From (20), (22), (40) and (A2), we can prove that

$$\dot{w}_s = \frac{1}{2}\mathbf{T}_s : \dot{\mathbf{C}}_s = \mathbf{S}_s : \dot{\mathbf{F}}_s = J_2 \boldsymbol{\sigma}_s : \mathbf{D}_s = A_{\lambda\gamma} A^{\beta\eta} T_\beta^\mu F_\eta^\gamma \dot{F}_\mu^\lambda + A^{\beta\gamma} T_\beta^\lambda F_\gamma^3 \dot{F}_\lambda^3. \tag{A3}$$

Appendix B. The generalized Young-Laplace equations

The Young-Laplace equations are used to describe the equilibrium conditions of a surface, which can be derived from the stationary condition of the functional proposed in Refs. [12,13]. The Lagrangian description of the Young-Laplace equations of the surface can be written as

$$\begin{aligned}
\mathbf{N} \cdot [\![\mathbf{S}]\!] \cdot \mathbf{N} &= -\left(\mathbf{S}_s^{(in)}\right) : \mathbf{b}_0 - \left[\mathbf{N} \cdot \left(\mathbf{S}_s^{(ou)}\right)\right] \cdot \nabla_{0s}, \\
\mathbf{P}_0 \cdot [\![\mathbf{S}]\!] \cdot \mathbf{N} &= -\left(\mathbf{S}_s^{(in)}\right) \cdot \nabla_{0s} + \left[\mathbf{N} \cdot \left(\mathbf{S}_s^{(ou)}\right) \cdot \mathbf{b}_0\right].
\end{aligned} \tag{B1}$$

where $[\![\mathbf{S}]\!]$ denotes the discontinuity of $\mathbf{S}$ across the surface A_0, $\mathbf{S}_s^{(in)}$ and $\mathbf{S}_s^{(ou)}$ are the in-plane term and the out-plane term of $\mathbf{S}_s$, respectively. The above equations have been given in [12], but some terms associated with $\mathbf{S}_s^{(ou)}$ were missing in Eqs. (35) and (36) in [12], and corrections have been made by Huang et al. [13].

The corresponding equations under the Eulerian description are [12]

$$\begin{aligned}\mathbf{n}\cdot[\![\boldsymbol{\sigma}]\!]\cdot\mathbf{n} &= -\boldsymbol{\sigma}_s:\mathbf{b},\\ \mathbf{P}\cdot[\![\boldsymbol{\sigma}]\!]\cdot\mathbf{n} &= -\boldsymbol{\sigma}_s\cdot\nabla_s\end{aligned} \tag{B2}$$

in which $\mathbf{P}=\mathbf{1}-\mathbf{n}\otimes\mathbf{n}$ is the corresponding perpendicular projection in the current configuration, $\boldsymbol{\sigma}$ is the Cauchy stress of the bulk, $[\![\boldsymbol{\sigma}]\!]$ denotes the discontinuity of $\boldsymbol{\sigma}$ across the surface A.

The operations of symbols ∇_{0s} and ∇_s can be found in [12,13].

References

[1] F. Bechstedt, Principles of Surface Physics, Springer-Verlag, Berlin, 2003.
[2] J.W. Gibbs, On the equilibrium of heterogeneous substances, in: J. Willard Gibbs (Ed.), The Scientific Papers of Thermodynamics, vol. 1, Dover, New York, 1961, pp. 55–353.
[3] R.C. Cammarata, K. Sieradzki, Effects of surface stress on the elastic moduli of thin films and superlattices, Phys. Rev. Lett. 62 (1989) 2005–2008.
[4] R. Carel, C.V. Thompson, H.J. Frost, Computer simulation of strain energy effects vs surface and interface energy effects on grain growth in thin films, Acta Mater. 44 (1996) 2479–2494.
[5] R. Shuttleworth, The surface tension of solids, Proc. Royal Soc. Lond. A 63 (1950) 444–457.
[6] W.D. Nix, H.J. Gao, An atomistic interpretation of interface stress, Scripta Mater. 39 (1998) 1653–1661.
[7] M.E. Gurtin, A. Ian Murdoch, A continuum theory of elastic material surfaces, Arch. Ration. Mech. An. 57 (1975) 291–323.
[8] A.I. Murdoch, Some fundamental aspects of surface modelling, J. Elasticity 80 (2005) 33–52.
[9] D.J. Steigmann, Elastic surface–substrate interactions, Proc. Royal Soc. A 455 (1999) 437–474.
[10] D.J. Steigmann, R.W. Ogden, Plane deformations of elastic solids with interinsic boundary elasticity, Proc. Royal Soc. A 453 (1997) 853–877.
[11] R. Dingreville, J. Qu, Interfacial excess energy, excess stress and excess strain in elastic solids: planar interfaces, J. Mech. Phys. Solids 56 (2008) 1944–1954.
[12] Z.P. Huang, J. Wang, A theory of hyperelasticity of multi-phase media with surface/interface energy effect, Acta Mech. 182 (2006) 195–210.
[13] Z.P. Huang, Z.Q. Wang, Y.P. Zhao, J. Wang, Influence of particle-size distribution on effective properties of nanocomposites, in: 2nd International Conference on Heterogeneous Materials Mechanics, Huangshan, China, 2008, pp. 925–932.
[14] A.I. Murdoch, Wrinkling induced by surface stress at boundary of an infinite circular-cylinder, Int. J. Eng. Sci. 16 (1978) 131–137.
[15] R.E. Miller, V.B. Shenoy, Size-dependent elastic properties of nanosized structural elements, Nanotechnology 11 (2000) 139–147.
[16] P. Lu, H.P. Lee, C. Lu, S.J. O'Shea, Surface stress effects on the resonance properties of cantilever sensors, Phys. Rev. B 72 (2005) 85405.
[17] J.G. Guo, Y.P. Zhao, The size-dependent elastic properties of nanofilms with surface effects, J. Appl. Phys. 98 (2005) 074306.
[18] J.G. Guo, Y.P. Zhao, The size-dependent bending elastic properties of nanobeams with surface effects, Nanotechnology 18 (2007) 295701.
[19] P. Sharma, L.T. Wheeler, Size-dependent elastic state of ellipsoidal nano-inclusions incorporating surface/interface tension, J. Appl. Mech. 74 (2007) 447–454.
[20] C.Q. Sun, Thermo-mechanical behavior of low-dimensional systems: the local bond average approach, Prog. Mater. Sci. 54 (2009) 179–307.
[21] M.E. Gurtin, A.I. Murdoch, Surface stress in solids, Int. J. Solids Struct. 14 (1978) 431–440.
[22] S. Cuenot, C. Frétigny, S. Demoustier-Champagne, B. Nysten, Surface tension effect on the mechanical properties of nanomaterials measured by atomic force microscopy, Phys. Rev. B 69 (2004) 165410.
[23] G.F. Wang, X.Q. Feng, Effects of surface elasticity and residual surface tension on the natural frequency of microbeams, Appl. Phys. Lett. 90 (2007) 231904.
[24] J. He, C.M. Lilley, Surface effect on the elastic behavior of static bending nanowires, Nano Lett. 8 (2008) 1798–1802.
[25] Z.Y. Ou, G.F. Wang, T.J. Wang, Effect of residual surface tension on the stress concentration around a nanosized spheroidal cavity, Int. J. Eng. Sci. 46 (2008) 475–485.
[26] Y. Cui, C.M. Lieber, Functional nanoscale electronic devices assembled using silicon nanowire building blocks, Science 291 (2001) 851–853.
[27] C.M. Lieber, Nanoscale science and technology: building a big future from small things, MRS Bull. 28 (2003) 486–491.
[28] C.M. Lieber, Z.L. Wang, Functional nanowires, MRS Bull. 32 (2007) 99–108.
[29] Z.P. Huang, L. Sun, Size-dependent effective properties of a heterogeneous material with interface energy effect: from finite deformation theory to infinitesimal strain analysis, Acta Mech. 190 (2007) 151–163.
[30] A. Hoger, On the determination of residual stress in an elastic body, J. Elasticity 16 (1986) 303–324.
[31] M.T. McDowell, A.M. Leach, K. Gall, Bending and tensile deformation of metallic nanowires, Model. Simul. Mater. Sci. 16 (2008) 045003.
[32] Y.D. Yan, J.J. Zhang, T. Sun, W.D. Fei, Y.C. Liang, S. Dong, Nanobending of nanowires: a molecular dynamics study, Appl. Phys. Lett. 93 (2008) 241901.
[33] C.Q. Chen, Y. Shi, Y.S. Zhang, J. Zhu, Y.J. Yan, Size dependence of young's modulus in ZnO nanowires, Phys. Rev. Lett. 96 (2006) 75505.
[34] G.Y. Jing, H.L. Duan, X.M. Sun, Z.S. Zhang, J. Xu, Y.D. Li, J.X. Wang, D.P. Yu, Surface effects on elastic properties of silver nanowires: contact atomic-force microscopy, Phys. Rev. B 73 (2006) 235409.
[35] L.D. Landau, E.M. Lifshitz, Theory of Elasticity, Butterworth-Heinemann, Boston, 1986.
[36] H.S. Park, P.A. Klein, 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 (2008) 3144–3166.