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Research paper

Surface effect in the bending of nanowires

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ABSTRACT

The surface effect in the bending of nanowires (nanobeams), including cantilever nanowires and fixed-fixed ones, is investigated in this paper with a recently developed elastic theory for nanomaterials, in which only the bulk surface-energy density and the surface-relaxation parameter are involved as two independent parameters to characterize the surface effect. Closed-form solutions of the maximum deflection and the effective elastic modulus in both kinds of nanowires are achieved. It is found that, comparing to the prediction of the classically elastic beam theory, the cantilever nanowire is softened, while the fixed-fixed one is stiffened by the surface effect in nanoscales, consistent well with the existing experimental measurements. Furthermore, an increasing aspect ratio of nanowires can further enhance the stiffening behavior of fixed-fixed nanowires and the softening behavior of cantilever ones, respectively. The present result should be helpful not only for explaining different surface effects in nanowires with different boundary conditions, but also for the design of nano-structures and nano-devices related to nanowires.

1. Introduction

The mechanical property of nanowires has attracted considerable interests due to their potential applications in nanostructures and nano-devices, such as sensors and resonators in nano-electro-mechanical systems (Craighead, 2000; Xie et al., 2012) and reinforcing phases in advanced nanocomposites (Lee et al., 2011; Gong et al., 2013). Similar to the other nanomaterials, nanowires have a size-dependently mechanical behavior due to a large surface-to-volume ratio (Liang and Upmanyu, 2005).

Static bending experiment has been widely adopted to explore the surface effect (size effect) in nanowires' elastic properties. The effective elastic modulus of fixed-fixed nanowires is found to increase with a decreasing diameter of nanowires (Cuenot et al., 2004; Chen et al., 2006; Jing et al., 2006; Tan et al., 2007; Chan et al., 2010; Celik et al., 2011). While for cantilever nanowires, the effective elastic modulus has an oppositely size-dependent behavior (Nam et al., 2006; Gavan et al., 2009; Sadeghian et al., 2009, 2010). All these experimental results provide us a direct understanding of the surface effect (size effect) in nanoscales.

Similar to the size effect in micro-scaled beam bending, which can not be predicted by the classical continuum mechanics, but depends on the strain gradient (for examples, Fleck and Hutchinson (1993, 1997); Gao et al., (1999); Chen and Wang (2000); Gao and Huang, (2001); Chen and Wang (2002), the classical beam theory is also invalid to predict the bending behavior of nanowires. Therefore, an elastic theory considering the surface effect (also addressed as size effect in nanoscales) in nanomaterials should be developed. Fortunately, based on the framework of the surface elasticity theory (Gurtin and Murdoch, 1975, 1978), many investigations on the size-dependently elastic behavior of nanowires have been carried out. Steigmann and Ogden (1997) and Chhapadia et al. (2011) introduced a surface flexural stiffness into the Gurtin–Murdoch (G-M) model in order to describe the curvature-dependent surface energy of bending nanowires. A similar method was also adopted by Chiu and Chen (2011). He and Lilley (2008) applied a generalized Young–Laplace (Y-L) model proposed by Wang and Feng (2007) to study the static bending behavior of nanowires, in which the effect of surface stress induced by a curvature was taken into account. Wang et al. (2010) modeled a bending nanowire as a core-shell composite system, which consists of a surface elastic layer and a core part. Song et al. (2011) improved the Y-L model by considering the in-plane surface stress tangential to the side surface of nanowires. Li et al. (2014) extended the Y-L model to the Timochenko nanobeam case. In addition, the molecular dynamics simulation method, as a major numerical approach, was also adopted to study the bending behavior of nanowires (Park et al., 2005; Chhapadia et al., 2011; Mohammadi and Sharma, 2012; Georgakaki et al., 2014).

The surface elasticity theory as well as its extensions has become a unique and popular model to investigate the surface effect

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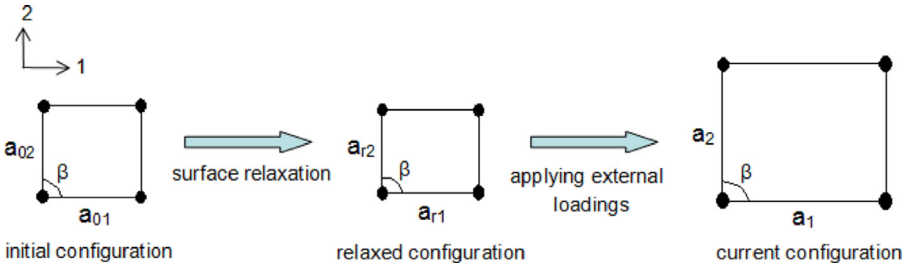

Fig. 1. Schematic of a surface unit cell in the initial (reference), relaxed and current configurations, where a local coordinate system (1, 2) coincides with the two bond directions.

in the mechanical behavior of nanowires. However, almost all the researchers can not avoid looking for the surface elastic constants involved in the surface elasticity theory, in order to give a precise comparison with the experimental result. Such a process is challenging because no experiment is valid to measure the surface elastic constant till now. Only a few molecular simulations can provide some numerical data (Miller and Shenoy, 2000; Shenoy, 2005; Mi et al., 2008; Chhapadia et al., 2011). Some physical problems of how to achieve the surface elastic constant in molecular simulations still exist and many factors will show significant influences on the numerical data. For example, how many atomic layers in a numerical model should be chosen as the surface of nanomaterials? Is the calculated surface elastic constant affected by the size of the numerical model or the potential energy function? The computational model is atomically continuous in molecular simulations, but an interruption exists between the surface layer and the inside part in most of the theoretical models. Furthermore, a negative value of the surface elastic constant is often found in the molecular simulations (Shenoy, 2005; Mi et al., 2008).

In view of the above problems, a new theory for nanomaterials has been developed recently within the framework of continuum mechanics (Chen and Yao, 2014), in which the surface elastic constant is no longer involved. Instead, a surface-induced traction to characterize the surface effect in nanomaterials is derived, which depends only on the Eulerian surface-energy density. Considering the relationship between the Eulerian surface-energy density and the Lagrangian one yields that only two kinds of material constants are needed in the new elastic theory, i.e., the bulk surface-energy density and the surface-relaxation parameter. The former is the surface energy density of a bulk solid while the latter is the ratio of the surface lattice length after and before a spontaneous surface relaxation (Ouyang et al., 2006; Chen and Yao, 2014).

In the present paper, the new theory is further used to analyze the surface effect in the bending of nanowires. Both a cantilever nanowire and a fixed-fixed one are investigated, in which closed-form solutions of the bending deflection and the effective elastic modulus of nanowires are given. Comparison of the theoretical prediction and the experimental result is carried out. The stiffening and softening mechanisms of nanowires with different boundary conditions are further discussed.

2. Brief introduction of the elastic theory for nanomaterials

An elastic theory to characterize the surface effect in nanomaterials was proposed by Chen and Yao (2014) recently, which was based on the surface energy density of nanomaterials. Assuming that a nano-solid has an idealized crystal structure, the initial state is regarded as a reference configuration, which will transform into a current one under an external loading. A Lagrangian coordinate system is attached to atoms on the surface with principal axes 1 and 2 parallel to the two basic vectors of a surface unit cell as shown in Fig. 1 (Nix and Gao, 1998). a_{01} and a_{02} represent lattice lengths in the two principal directions, respectively. β denotes an angle between the two basic vectors. Due to a spontaneous surface relaxation, two lattice lengths become a_{r1} and a_{r2}, respectively. Both of them further change to be a_1 and a_2 in the current configuration when an external loading is added on the nano-solid.

The potential energy function Π of the nano-solid in the current configuration can be written as

$$\Pi(\mathbf{u}) = \int_{V-S} \psi(\varepsilon) dV + \int_S \phi dS - \int_{V-S} \mathbf{f}\cdot\mathbf{u} dV - \int_{S_p} \mathbf{p}\cdot\mathbf{u} dS \tag{1}$$

where ψ is the elastic strain energy density, ϕ is the Eulerian surface-energy density in the current configuration, $\mathbf{f}$ and $\mathbf{p}$ are the body force and external surface traction, respectively. $\mathbf{u}$ and $\boldsymbol{\varepsilon}$ are the displacement and strain induced by $\mathbf{f}$ and $\mathbf{p}$. V and S denote the volume and the surface of the nano-solid.

The variation analysis of Eq. (1) yields the following equilibrium equation and stress boundary conditions,

$$\begin{cases} \boldsymbol{\sigma}\cdot\nabla + \mathbf{f} = 0 \,(\text{in}\, V-S) \\ \mathbf{n}\cdot\boldsymbol{\sigma}\cdot\mathbf{n} = \mathbf{p}\cdot\mathbf{n} - \gamma_n \mathbf{n} (\text{on}\, S) \\ (\mathbf{I}-\mathbf{n}\otimes\mathbf{n})\cdot\boldsymbol{\sigma}\cdot\mathbf{n} = (\mathbf{I}-\mathbf{n}\otimes\mathbf{n})\cdot\mathbf{p} - \gamma_t \,(\text{on}\, S) \end{cases} \tag{2}$$

where $\boldsymbol{\sigma}$ is the bulk Cauchy stress tensor, ∇ is a spatial gradient operator in the current configuration, $\mathbf{n}$ is the unit normal vector perpendicular to the surface S of the nano-solid, $\mathbf{I}$ is a unit tensor; γ_n and $\boldsymbol{\gamma}_t$ are the normal and tangential components of an additionally surface-induced traction vector, respectively, which characterizes a force disturbance at boundaries due to the surface effect. Based on an infinitesimal element, the virtual work method yields the surface-induced traction as (Chen and Yao, 2014),

$$\gamma_t = \nabla_s\phi,\ \gamma_n\mathbf{n} = \phi\left(\frac{1}{R_1}+\frac{1}{R_2}\right)\mathbf{n} = \phi(\mathbf{n}\cdot\nabla_s)\mathbf{n} \tag{3}$$

where ∇_s is a surface gradient operator in the current configuration, R_1 and R_2 are the two principal radii of curvature of a curved surface.

Relation between the Eulerian surface-energy density ϕ and the Lagrangian surface energy density ϕ_0 satisfies

$$\phi = \frac{\phi_0}{J_s} \tag{4}$$

where J_s is a Jacobean determinant characterizing the surface deformation from the reference configuration to the current one. Eq. (4) can also be found in Nix and Gao (1998) and Huang and Wang (2006).

Thus, the equilibrium equations can be rewritten as (Chen and Yao, 2014),

$$\begin{cases} \boldsymbol{\sigma}\cdot\nabla + \mathbf{f} = 0 \,(\text{in}\, V-S) \\ \mathbf{n}\cdot\boldsymbol{\sigma}\cdot\mathbf{n} = \mathbf{p}\cdot\mathbf{n} - \dfrac{\phi_0(\mathbf{n}\cdot\nabla_s)}{J_s} \,(\text{on}\, S) \\ (\mathbf{I}-\mathbf{n}\otimes\mathbf{n})\cdot\boldsymbol{\sigma}\cdot\mathbf{n} = (\mathbf{I}-\mathbf{n}\otimes\mathbf{n})\cdot\mathbf{p} + \dfrac{\phi_0(\nabla_s J_s)}{J_s^2} - \dfrac{\nabla_s\phi_0}{J_s} \,(\text{on}\, S) \end{cases} \tag{5}$$