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A finite element modeling for large deflection analysis of uniform and tapered nanowires with good interpretation of experimental results

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ABSTRACT

A large deflection model of nanowires with surface effects is presented. The surface effects are modeled via the generalized Young–Laplace equation. Shear deformation is introduced by using the Timoshenko beam theory, and the total Lagrangian finite element formulation is used for the numerical solution of the problem. To the mathematical model be consistent with the support properties used in the reference experiments, some realizations are considered in the modeling of the supports. The agreement between the results of the proposed model and the experimental measurements reported in the literature is very good as it is much better from the correspondence between the results of the previous models and the experimental results. Besides, at the first time, the large deformation analysis of tapered nanowires is employed, and the numerical results are tabulated.

1. Introduction

Nanowires have several applications as actuators and sensors in nanoelectromechanical systems [1–4]. Accordingly, predicting mechanical responses of nanowires is important for the design of these systems. Conventionally, bending tests are used for determining mechanical properties of materials at the nanoscale [5–7]. Usually, the properties of nanowires are determined by the correspondence between the test results and an appropriate mathematical model. Without an appropriate mathematical model, the study of deformation of nanowires with different geometries and loading conditions are time consuming and expensive. Hence, several researchers have proposed different analytical and numerical models to simulate the deformation of nanowires under different setting and conditions.

When the dimensions of a structure come close to the nanoscale, the classical continuum theories cannot accurately predict the deformation behavior of the structure. In modeling of the nanostructures, media may be assumed discrete or continuous. The methods based on discrete assumption, such as molecular dynamics methods [8,9] are computationally expensive. So, more researchers attempt to use modified continuum theories for modeling of nanostructures. According to high surface to volume ratio in the nanowires, continuum theories with the surface effects are proposed as a modification of the classical continuum theories for modeling of these nanostructures.

In the analysis of a nanowire using the continuum theories containing the surface effects, the nanowire is considered as a collection of a bulk material and its surfaces, where they have different material properties. The bulk and its surfaces have stress interactions to lead continuous deformations.

Gurtin and Murdoch [10–12] presented a continuum theory for elastic material surfaces, and Cammarata [13–15] considered the surface effects in similar to Gurtin–Murdoch theory via the generalized Young–Laplace equation.

Afterwards, many researchers have analyzed deflections of nanowires with considering the surface effects. In most works, the small deflections of nanowires have been studied [16–21]. However, in some applications nanowires bear large deflections [22,23].

Zeng and Zheng [24] developed a large deflection theory of nanobeams by considering different material properties for the surface and the bulk associated to each nanobeam. They ignored the surface stress at all. He and Lilley [25] presented a model for analyzing the large deformation of nanowires with the surface stress effect. They used the finite element absolute nodal

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coordinate formulation in order to model the large deformation of a nanowire. Liu et al. [26] studied the static large displacement bending of a nanowire with considering the surface effects. They developed a computer program based on the shooting method to numerically solve the supplementary nonlinear equations. In most of these works [25–27], the surface effects are modeled via the generalized Young–Laplace equation. Sapsathiarn and Rajapakse [28] also presented a model for the large deflections of a nanobeam. In this model, the surface energy effects were accounted through Gurtin–Murdoch continuum theory and the globally adaptive numerical quadrature scheme was used for the solution.

In all of the works mentioned above [24–28], shear deformations were neglected, and the large deflection analyses of a nanowire were based on Euler–Bernoulli beam theory. The experiments have shown that this theory gives reasonable results when the length to the height ratio of a nanowire to be larger than 10 [27]. The shear deformations are accounted for in the Timoshenko beam theory. Therefore, this theory gives more accurate results, especially when the nanowire is relatively thick.

In the present study, the Timoshenko beam theory together with the generalized Young–Laplace equation is used to model the large deflection response of nanowires. The total Lagrangian finite element formulation is employed for the numerical solution of the problem. The finite element method allows us to model the nanowires with non-uniform cross sections and arbitrary loadings and boundary conditions.

Among the large deflection analysis of nanowires presented in the references above, the Ref. [28] is the only work in which the numerical results are compared with the experimental measurements [23].

In the present work, the obtained numerical results are verified by the large deflection measurements of Ref. [23]. Also, for the first time, the numerical results are compared with the extremely large deflection measurements of a nanowire reported in Ref. [22]. Furthermore, a proper interpretation of the experimental results is proposed based on the properties of the experimental setup used in the experiments.

The present article is organized as follows: In Section 2, the large deflection model of a nanowire with the surface effects is introduced. This model is based on the Timoshenko beam theory and the total Lagrangian finite element formulation. In Section 3, several numerical results are presented and discussed. Initially, the developed finite element code is verified by comparison of the related results with the experimental measurements of a steel macro beam. Next, the model is used to interpret the experimental results obtained in deflections of a chromium cantilever nanowire. At the end of this section, the numerical results of the present model in the large deflection analyses of a tapered silver nanowire with sinusoidal distributed loads are presented.

2. Mathematical modeling

In the present work, a computer code has been written for the large deformation analysis of a nanowire with considering the surface effects. The code is based on the total Lagrangian finite element formulation of a Timoshenko beam. The formulation has been modified to take into account the surface effects in nanowires. In this section, the theory of the surface effects in nanowires are presented first. Then the mathematical formulation for the large deflection of a Timoshenko beam is explained. Next, the total Lagrangian finite element formulation employed for the numerical solution of the problem is illustrated. Also, the modifications of the numerical model for the inclusion of the surface effects are clarified.

2.1. The surface effects

The surface effects in a nanowire are modeled by a modified continuum theory via the generalized Young–Laplace equation. In this model, the nanowire is considered as combination of a core or bulk and its surfaces, so that the bulk and its surfaces have different properties with stress interactions and continuous deformations. Based on the theory of Cammarata [13], the surface stress tensor $\tau_{\alpha\beta}$ is related to the surface energy density γ as

$$\tau_{\alpha\beta} = \gamma\delta_{\alpha\beta}+\frac{\partial\gamma}{\partial\varepsilon_{\alpha\beta}}, \tag{1}$$

where $\varepsilon_{\alpha\beta}$ is the surface strain tensor. For nanowires, Eq. (1) can be written in one-dimensional form as [17]

$$\tau = \tau_0+E_s\varepsilon, \tag{2}$$

where τ_0 is the residual surface stress and E_s is the surface elastic modulus.

The stress interaction between the surface and the bulk is introduced in the model with the generalized Young–Laplace equation. According to the generalized Young–Laplace equation [14,17,29], the surface stress causes a jump of the normal stress across the surface, i.e.,

$$\left\langle \sigma_{ij}^{+}-\sigma_{ij}^{-}\right\rangle n_i n_j=\tau_{\alpha\beta}\kappa_{\alpha\beta}, \ (i, j=1, 2, 3; \alpha, \beta=1, 2) \tag{3}$$

where σ_{ij}^{+} and σ_{ij}^{-} are symbols for the stresses above and below the solid surface, respectively. The symbol n_i is the unit vector normal to the surface, $\tau_{\alpha\beta}$ is the surface stress tensor and $\kappa_{\alpha\beta}$ is the curvature tensor. For a nanowire with large deformation, the stress jump will lead to a distributed load q_s, perpendicular to the neutral axis of the nanowire through the entire length as it is shown in Fig. 2.1, namely as

$$q_s = H\kappa_\theta, \tag{4}$$

where κ_θ is the curvature of the neutral axis of the nanowire that defined by the derivative of θ (the slope of the neutral axis of the nanowire) with respect to X i.e.,

$$\kappa_\theta = \theta', \tag{5}$$

and H is a constant parameter determined by the shape of the cross section and the residual surface stress, given by

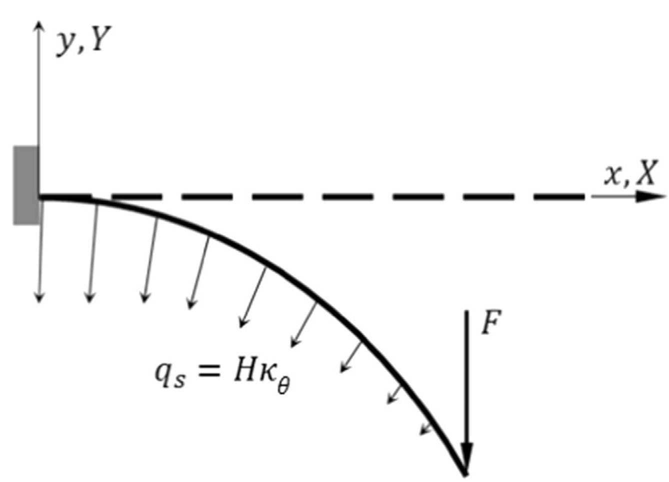

Fig. 2.1. The illustration of the distributed load due to the positive residual surface stress that is perpendicular to the neutral axis through the entire length of the nanowire under a vertical point load.