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Progress in Natural Science: Materials International 25 (2015) 520–524
Progress in Natural Science Materials International
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Letters

Surface effects on static bending of nanowires based on non-local elasticity theory

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Received 2 July 2015; accepted 1 August 2015
Available online 4 November 2015

Abstract

The surface elasticity and non-local elasticity effects on the elastic behavior of statically bent nanowires are investigated in the present investigation. Explicit solutions are presented to evaluate the surface stress and non-local elasticity effects with various boundary conditions. Compared with the classical Euler beam, a nanowire with surface stress and/or non-local elasticity can be either stiffer or less stiff, depending on the boundary conditions. The concept of surface non-local elasticity was proposed and its physical interpretation discussed to explain the combined effect of surface elasticity and non-local elasticity. The effect of the nanowire size on its elastic bending behavior was investigated. The results obtained herein are helpful to characterize mechanical properties of nanowires and aid nanowire-based devices design.

Keywords: Surface effect; Non-local elasticity; Nanowires; Size effect; Euler–Bernoulli beam

1. Introduction

Outstanding mechanical properties of nanowires have been of considerable interest to researchers. For example, Wu et al. [1] measured the yield strength of Au nanowires by three-point bending using atomic force microscopy (AFM), and it's average values are 5.6 ± 1.4 GPa, which is more than 25 times higher than the bulk Au values. Treacy et al. [2] found that the Young's modulus of carbon nanotubes was in the Tera-Pascal (TPa) range. Cuenot et al. [3] reported the diameter-dependent elastic modulus effects in Ag and Pb nanowires. Meanwhile, the classical beam theory has been unsuccessful to theoretically analyze the mechanical properties of one-dimensional nano-materials. Hence, accurate description of nanowires' mechanical behavior is essential.

Surface effects have been recognized as significant factors during the deformation process of nanobeams. Chen et al. [4] proposed a core–shell composite nanowires model to explain the surface effects on the mechanical behavior of nanowires. He et al. [5] investigated surface stress and surface elasticity effects on the elastic behavior of statically bent nanowires. Jiang et al. [6] addressed combined surface and shear deformation effects based on the Timoshenko beam theory and the Young–Laplace equation. Wang and Feng [7] studied surface effects on buckling and vibration behavior of nanowires. All these research reports show that the surface effects play a significant role in the deformation behavior of one-dimensional nano-materials.

Based on the lattice dynamics theory and experimental observations on phonon dispersion, Eringen [8,9] proposed the non-local elasticity theory in 1972. According to this theory, it is assumed that the stress at a given reference point depends not only on the strain at this point, but also on the strain at other points in the body. This way, the influence of the long range forces between the atoms is taken into consideration, and thus the internal size scale can be introduced in the constitutive equations. In recent years, many researchers have successfully applied the non-local elasticity theory for explaining the deformation behavior of micro- and nanobeams [10–13].

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Peer review under responsibility of Chinese Materials Research Society.

http://dx.doi.org/10.1016/j.pnsc.2015.09.012
1002-0071/

In this letter, the non-local elasticity theory is implemented to analyze the bending behavior of centrally loaded nanowires with consideration of surface elasticity and surface stress.

2. Non-local elasticity and surface effects

Under certain conditions, based on the non-local elasticity theory, the non-local stress tensor, σ_{xy}, within a two-dimensional region, using the Green's functions, is expressed as [8]:

$$\sigma'_{xy} = \left[1-(e_0 l)^2\nabla^2\right]\sigma_{xy}, \quad (1)$$

where σ'_{xy} is the (classical) stress tensor, l represents internal characteristic length (e.g., the lattice parameter, grain size, C–C bond length, etc.). The Laplace operator ∇^2 equals $\partial^2/\partial x^2+\partial^2/\partial y^2$ in Cartesian coordinates, and e_0 is a constant appropriate to each material. Eringen [8] obtained the magnitude of $e_0=0.39$ by matching the dispersion curves of the plane waves with those of atomic lattice. Hence, the Hooke's law for uniaxial stress state can be expressed as:

$$\sigma(x)-(e_0 l)^2\frac{\partial^2\sigma(x)}{\partial x^2} = E\epsilon(x) \quad (2)$$

Since the surface-to-volume ratio is large in nano-materials, nanowires were treated as a superposition of the surface layers and the bulk volume. The thickness of the beam is much larger than the thickness of the surface layer t_0. This way, the traditional flexural rigidity D for the bulk material is replaced by the effective flexural rigidity $D*$ for the composite beam. The effective flexural rigidity $D*$ for either rectangular or circular cross-section is:

$$D* = \begin{cases} \frac{Eab^3}{12}+\frac{E_s ab^2}{2}+\frac{E_s b^3}{6} & \text{(rectangle)} \\ \frac{\pi E d^4}{64}+\frac{\pi E_s d^3}{8} & \text{(circular)} \end{cases}, \quad (3)$$

where a is the length of rectangle, b represents the width of rectangle, d is the diameter of circular, E and E_s represent the Young's modulus of the bulk and the surface, respectively.

The existing constant residual surface tension on the surfaces above and below the bulk material causes a nanobeam to curve. The mathematic relation between the curvature tensor κ and the stress jump $\left\langle \tau^+_{ij}-\tau^-_{ij}\right\rangle$ across a surface is based on the generalized Laplace–Young equation [5,6,14]:

$$\left\langle \tau^+_{ij}-\tau^-_{ij}\right\rangle n_i n_j = \tau_s\kappa, \quad (4)$$

where τ^+_{ij} and τ^-_{ij} denote the upper and the lower surface stresses, respectively, n_i is the unit normal vector to the surface, κ is the curvature tensor of the nanowire and τ_s is the surface stress tensor given by [5,6,15]:

$$\tau_s = \tau_0 + E_s\varepsilon_x, \quad (5)$$

where τ_0 is the residual surface stress along the longitudinal direction of the nanobeam and ε_x is the strain along the nanowire longitudinal direction.

According to Eq. (4), the stress jump leads to a distributed transverse force $q(x)$ along the nanowire longitudinal direction [14]. For a deformed nanowire, the distributed force is given by [5,6]:

$$q(x) = Hw''(x), \quad (6)$$

where $w(x)$ denotes the nanobeam transverse displacement, and H is a constant parameter given by [5,6]:

$$H = \begin{cases} 2\tau_s a & \text{(rectangle)} \\ 2\tau_s d & \text{(circular)} \end{cases} \quad (7)$$

3. Non-local elasticity and surface stress coupling effects on the Euler–Bernoulli beam

Considering the Euler–Bernoulli beam model, the equilibrium equations for the shear force, T, the bending moment, M, and the transverse distributed load, $q(x)$, are:

$$\frac{\partial T}{\partial x}+q(x)=0 \quad (8)$$

$$T-\frac{\partial M}{\partial x}=0 \quad (9)$$

The bending moment constitutive relation accounting for the non-local elasticity and surface stress effects is written as:

$$M-(e_0 l)^2\frac{\partial^2 M}{\partial x^2} = -D^*\frac{\partial^2 w}{\partial x^2} \quad (10)$$

In view of Eqs. (8)–(10), the governing equation for the bending of non-local Euler–Bernoulli beam with the surface effects is given by

$$D^*\frac{\partial^4 w}{\partial x^4}+(e_0 l)^2\frac{\partial^2 q(x)}{\partial x^2}-q(x)=0 \quad (11)$$

By substituting Eq. (6) into Eq. (11), one obtains

$$\left[D^*+H(e_0 l)^2\right]\frac{\partial^4 w}{\partial x_4} = H\frac{\partial^2 w}{\partial x^2} \quad (12)$$

Letting

$$\eta^E_{ns} = \frac{HL^2}{D^*+H(e_0 l)^2} \quad (13)$$

The boundary conditions for the two kinds of the end are:

$$\text{Clamped end}: w(0)=0, w'(0)=0 \quad (14)$$

$$\text{Simply supported end}: w(0)=0, w''(0)=0 \quad (15)$$

Fig. 1 shows the deformation of a nanobeam with surface stress in different boundary conditions. As a constant concentrated force P is loading the free end at $x=L$, the moment and the force equilibrium conditions of the clamped-free beam (C-F) are:

$$-M(0) = PL+\int_0^L Hw''(x)x\,dx = PL+HLw'(L)-Hw(L) \quad (16)$$

and

$$T(0) = P+\int_0^L Hw''(x)dx = P+Hw'(L)-Hw'(0), \quad (17)$$

respectively. When the simply supported beam (S-S) subjected to a concentrated force P at the midpoint $x=L/2$, the slope at $x=L/2$

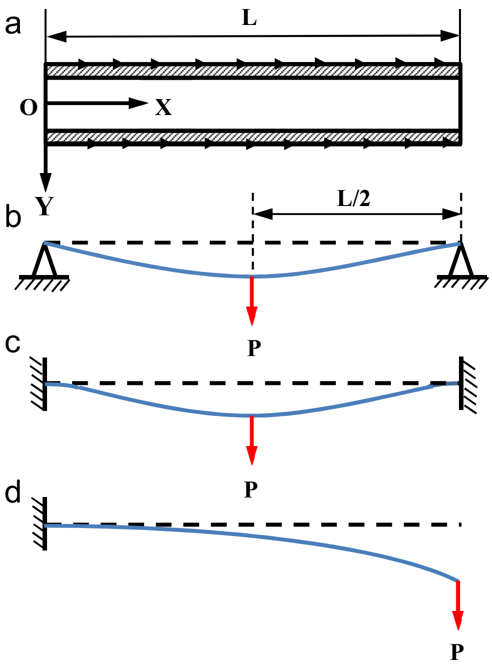

Fig. 1. (a) Illustration of a nanobeam with surface stress. Deformation of a nanowire with different boundary conditions: (b) simply supported; (c) clamped–clamped; (d) clamped-free.

is zero due to symmetry, resulting in

$$w'\left(\frac{L}{2}\right)=0 \tag{18}$$

and the force equilibrium condition at $x=0$ is

$$T(0)=\frac{P}{2}+\int_0^{\frac{L}{2}} Hw''(x)dx=\frac{P}{2}-Hw'(0) \tag{19}$$

For the clamped–clamped nanowire (C-C), a constant concentrated force P is applied at the midpoint $x=L/2$. At $x=0$, when the C-C nanowire boundary conditions are equal to those of the cantilever beam, the slope is identical with the simply supported beam at $x=0$, and the force equilibrium condition at $x=0$ is

$$T(0)=\frac{P}{2}+\int_0^{\frac{L}{2}} Hw''(x)dx=\frac{P}{2} \tag{20}$$

The solution to Eq. (11) with different boundary conditions and concentrated force is written as:

$$w(x)=\begin{cases}\frac{P}{2H}\left[x-\frac{L}{\sqrt{\eta_{ns}^E}}\frac{\sinh\left(\frac{\sqrt{\eta_{ns}^E}}{L}x\right)}{\cosh\left(\frac{\sqrt{\eta_{ns}^E}}{2}\right)}\right], x\in\left[0,\frac{L}{2}\right] & (\mathrm{S-S})\\ \frac{P}{2H}\left[x-\frac{L}{\sqrt{\eta_{ns}^E}}\tanh\left(\frac{\sqrt{\eta_{ns}^E}}{4}\right)-\frac{L}{\sqrt{\eta_{ns}^E}}\frac{\sinh\left(\frac{\sqrt{\eta_{ns}^E}}{L}x-\frac{\sqrt{\eta_{ns}^E}}{4}\right)}{\cosh\left(\frac{\sqrt{\eta_{ns}^E}}{4}\right)}\right], x\in\left[0,\frac{L}{2}\right] & (\mathrm{C-C})\\ \frac{P\cosh\sqrt{\eta_{ns}^E}}{H}\left[x-\frac{L}{\sqrt{\eta_{ns}^E}}\tanh\sqrt{\eta_{ns}^E}-\frac{L}{\sqrt{\eta_{ns}^E}}\frac{\sin\left(\frac{\sqrt{\eta_{ns}^E}}{L}x-\sqrt{\eta_{ns}^E}\right)}{\cosh\left(\sqrt{\eta_{ns}^E}\right)}\right], x\in[0,L] & (\mathrm{C-F})\end{cases} \tag{21}$$

When the effects of non-local elasticity are neglected, the non-local parameter e_0l is equal to zero, and Eq. (21) are reduced to the solutions in Ref. [5]. When the surface effects are neglected, the solutions are demonstrated in Ref. [11]. When both the non-local elasticity and the surface effects are neglected, the general solution with different boundary conditions is expressed as:

$$w(x)=\begin{cases}\frac{P(3L^2-4x^2)x}{48D^*}, x\in\left[0,\frac{L}{2}\right] & (\mathrm{S-S})\\ \frac{P(3L-4x)x^2}{48D^*}, x\in\left[0,\frac{L}{2}\right] & (\mathrm{C-C})\\ \frac{P(3L-x)x^2}{6D^*}, x\in[0,L] & (\mathrm{C-F})\end{cases} \tag{22}$$

4. Results and discussion

To study the effects of surface stress and non-local elasticity during the deformation behavior of the Euler–Bernoulli beam in bending, we used the same parameters as in He's [5] work: $d=50$ nm, $E=76$ GPa, $\tau_s=1$ μN/μm and $E_s=0$. The non-local parameter e_0l is assumed to be 80 nm and the beam length is 1000 nm.

Fig. 2 shows the displacement profile of different nanowire models based on the classical Euler–Bernoulli beam theory subjected to the same concentrated load with the non-local elasticity and surface stress coupling effect, only with the non-local elasticity effect, only with the surface stress effect and without any effects. All effects have a significant influence on the static displacement of nanowires with different boundary conditions. Due to the surface stress effect, the C-F nanobeam exhibits less stiff behavior, while the S-S and the C-C nanobeams are stiffer. This phenomenon is due to the signs of the curvature and surface stress, which cause an additional distributed load and change the nanowire stiffness. For the C-F nanobeam a positive curvature results in a positive distributed transverse force, which increases the transverse bending displacement. For the S-S nanobeam the negative curvature results in negative distributed transverse force which decreases the transverse bending displacement. For the C-C nanobeam the negative curvature plays more important role than positive curvature when $\tau_0>0$. The result we obtained has a similar trend in comparison with the work of others [6]. Owing to the non-local elasticity effect, the S-S and C-C nanobeams show less stiff behavior, while the C-F nanobeam is the same as the classical Euler–Bernoulli beam, which has been clearly discussed by Reddy [16]. Considering the non-local continuum theory, the interaction of the long range forces between the atoms of a nanobeam increases the transverse bending displacement, which exhibits lower stiffness. The combined effects of the surface stress and non-local elasticity result in even stiffer behavior compared with the single effect in the S-S and C-C nanobeams. At the same time, the C-F nanobeam with the combined effects shows less stiff behavior compared with the classical Euler beam, but stiffer than the nanobeam with the surface stress effect.

The surface effect is based on the core–shell composite model. Therefore, a nanowire can be divided into two parts: the core, which has the same properties as the bulk, and the shell or the surface, which has different properties due to the surface stress. That also means that the atoms arrangement between the core and the surface is different. The non-local elasticity theory is aimed at studying the interaction of the long range forces between the atoms

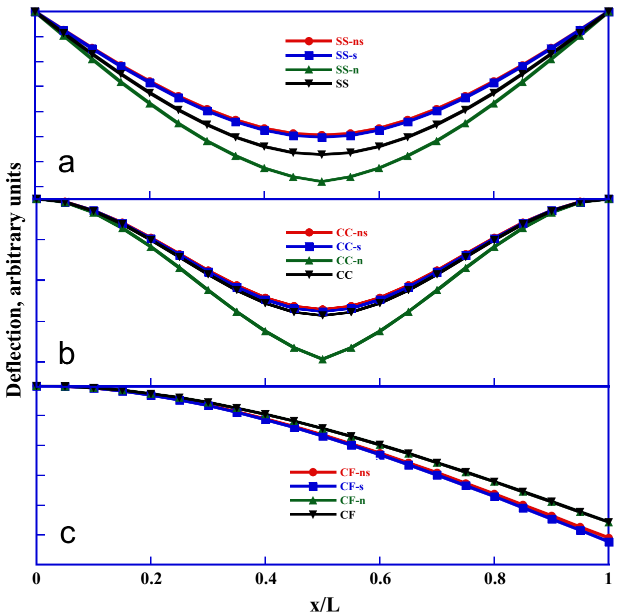

Fig. 2. Transverse displacement along the nanowire longitudinal direction with different boundary conditions: (a) simply supported; (b) clamped-clamped and (c) clamped-free. The red line represents the coupling effect, the blue line – the surface stress effect, the green line – non-local elasticity effect, and the black line – the classical Euler–Bernoulli beam theory.

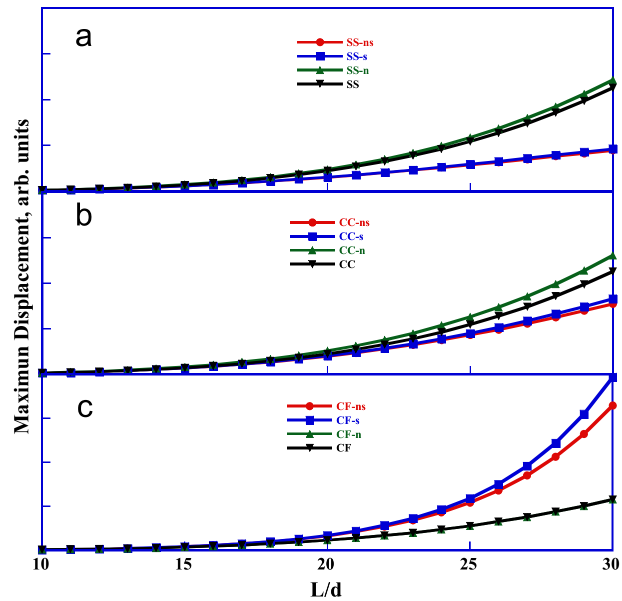

Fig. 3. Variation of the maximum static displacements by varying the *L/d* aspect ratio for: (a) simply supported; (b) clamped–clamped and (c) Clamped-free nanowires. The red line represents the coupling effect, the blue line – the surface stress effect, the green line – non-local elasticity effect, and the black line – the classical Euler–Bernoulli beam theory.

by assuming that the stress at a given reference point depends not only on the strain at this point, but also on the strain at other nearby points. Thus, the different atoms arrangement could cause different interaction of the long range forces. We define the long range interaction forces of the surface atoms using surface non-local elasticity. It can be seen that the surface non-local elasticity and not the bulk non-local elasticity plays a significant role in the nanowire bending deformation.

To study the nanowire size effect on its bending behavior, the diameter of nanowires was varied and its length was fixed at 1000 nm to observe the maximum displacement. The results in Fig. 3 show that when the *L/d* aspect ratio is relatively small, the effects of the surface stress and non-local elasticity can be neglected. As the aspect ratio gets relatively larger, the surface stress effect decreases the maximum displacement significantly, while the non-local elasticity effect slightly increases the beam displacement for the S-S and C-C boundary conditions. The surface non-local elasticity effect has even greater impact on the bending deformation behavior than the surface elasticity effect as the aspect ratio increases. For the C-F nanobeam, the non-local elasticity has no obvious effect on the bending behavior when the end force is applied to the beam, as proven by Wang [11]. But at the same time, the surface nonlocal elasticity effect can affect the maximum displacement as the aspect ratio increases. The difference between non-local surface and surface elasticity is due to the effects of long range forces between the surface atoms.

5. Conclusions

The surface stress effect, non-local elasticity effect and their coupling were investigated for the bending deformation behavior based on the Euler–Bernoulli beam theory. The surface non-local elasticity plays a more important role than the bulk elasticity in the coupling effect at the nano-scale. Static bending results show that nanowires can be either stiffer or less stiff, or do not change at all compared with the classical Euler–Bernoulli beam, depending on the boundary conditions. When the structure size is at the nanometer scale, the surface stress, non-local elasticity and the coupling effects have a significant impact on the deformation behavior of nanowires. This work is meaningful in relation to the applications of nanowires and development of basic elements of the nano-electro-mechanical systems.

Acknowledgments

This study was supported by the National Basic Research Program of Chian (Grant no. 2012CB937502), by the National Science Foundation (IRES1358088), and by the National High Technology Research and Development Program of China (863 Program) (Grant no. 2011AA050305).

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