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Paper for control

SURFACE EFFECTS ON AXIAL BUCKLING OF NONUNIFORM NANOWIRES USING NONLOCAL ELASTICITY THEORY

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The nonlocal elasticity theory is used to study the buckling behavior of a nonuniform nanowire with consideration of surface effects. An analytical expression for the calculation of critical buckling load of the nanowire is obtained. The expression can be simplified to analyze the critical buckling load of the nanowire with uniform cross section, and the analyzed result agrees with the previous work. In addition, the Rayleigh-Ritz method is used to analyze the influences of surface and nanolocal effects on the critical buckling load of the nonuniform nanowire. Results show that the surface effects are more significant for a slender nanowire with a higher diameter ratio. The critical buckling load decreases with increasing nonlocal parameter.

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1. Introduction

Nanowires have been of significant interest to researchers because they have a wide range of potential applications in nanoelectromechanical systems and biotechnology.[1-2] For nanoscale materials, due to high surface-to-volume ratio, surface effects become important and can influence their physical and chemical properties. Accordingly, much theoretical and experimental work has been done in recent years to investigate the surface effects on nanowires.[3-7] For example, Chen et al. [3] experimentally measured the Young's modulus of ZnO nanowire and found that the surface effects on the elastic property of the nanowire are significant. He and Lilley [5] studied the surface effects on the elastic behavior of static bending nanowires using the Euler beam theory.

Recently, Song et al. [8] developed a high-order continuum model to investigate high-frequency wave propagation in nanowires with surface effects. Zheng et al. [9] utilized the core–shell model to study the surface effect on the elastic property of nanowires and found that the influence of surface elasticity on the elastic moduli can be well characterized by two dimensionless material and geometric parameters.

In addition, some researchers studied the buckling properties of nanowires. For example, Wang et al. [10] studied the buckling behavior of GaN nanowires under uniaxial compression using molecular dynamic simulation. Wang and Feng [11] derived an analytical expression for the axial buckling of nanowires with consideration of surface effects and analyzed the buckling behavior of nanowires subjected to surface elasticity and residual surface tension.

The cross-section of nanowires in the theoretical analysis of the above papers was assumed to be uniform. The nanowires fabricated, however, are often tapered instead of uniform cross-section. [12-13] In this article, the nonlocal elasticity theory is used to analysis the buckling behavior of nonuniform nanowires with consideration of surface effects. The nonlocal elasticity theory is a modified classical elasticity theory. [14-15] This theory with long-range interactions revealing the nano-scale effect on the response of structures is often applied to analyze the mechanical behaviours of nanomaterials. [16-19] In addition, the effects of nonlocal parameter and surface tension on the buckling of the nonuniform nanowires are investigated.

2. Analysis

A schematic diagram of a cantilever nanowire with nonuniform cross-section is subjected to a uniaxial compression P as depicted in Fig. 1. The nanowire diameter is linearly varied with its length L and has the Young's modulus E and volume density ρ. The maximum diameter at the fixed end is D_0 and the minimum diameter at the free end is D_1. In this work, the surface and small scale effects on the buckling of the nanowire are studied by using the nonlocal elastic theory. The analysis for the surface effects is considered as a uniform surface layer with infinitesimal thickness.[20]

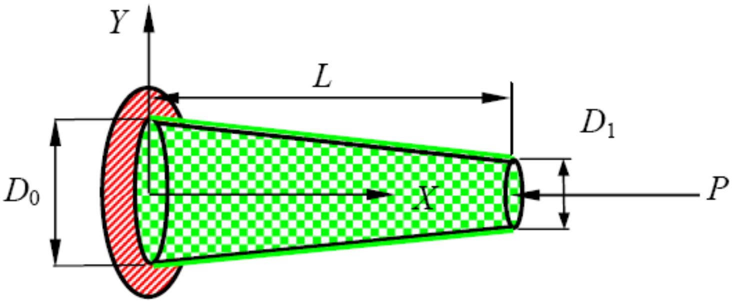

Fig. 1. A cantilever nanowire with a varying diameter and a uniform surface layer.

The nonlocal constitutive relations for one-dimensional case can be written as [15]

$$M-(e_0a)^2\frac{d^2M}{dX^2}=-E^*I^*\frac{d^2Y}{dX^2} \tag{1}$$

where Y is transverse displacement depends on the spatial coordinate along the longitudinal axis X; M is the resultant bending moment, E^*I^* is the effective flexural rigidity which includes the surface bending elasticity and bending rigidity [11], and e_0a is the nonlocal constant which is used to modify the classical elasticity theory and is limited to apply to a device on the nanometer scale.

In addition, based on the Euler beam theory, the equation of buckling for a nanowire is expressed by

$$V=(P-H)\frac{dY}{dX} \tag{2}$$

$$V=\frac{dM}{dX} \tag{3}$$

where V is the is the resultant shear force, H is the constant parameter which is determined by the residual surface tension, and P is the axial compression force.
Using Eqs.(1)-(3), the nonlocal bending moment M can be expressed as:

$$M=-E^*I^*\frac{d^2Y}{dX^2}+(e_0a)^2\frac{d}{dX}[(P-H)\frac{dY}{dX}] \tag{4}$$

Therefore, the governing equation of buckling for the nonuniform nanowire with consideration of both surface and nonlocal effects can be expressed as

$$\frac{d^2}{dX^2}(E^*I^*\frac{d^2Y}{dX^2})+[1-(ea_0)^2\frac{d^2}{dX^2}][\frac{d}{dX}(P-H)\frac{dY}{dX}]=0 \tag{5}$$

The diameter $D(X)$ of the nanowire varies linearly along the longitudinal axis X. Here, the parameters $E^*I^*(X)$ and $H(X)$ are defined as [11]

$$E^*I^*(X)=\frac{E}{64}\pi D(X)^4+\frac{E^S}{8}\pi D(X)^3 \tag{6}$$

$$H(X)=2\tau D(X) \tag{7}$$

where E^S and τ are the surface elasticity modulus and residual surface tension of the nanowire per length, respectively.

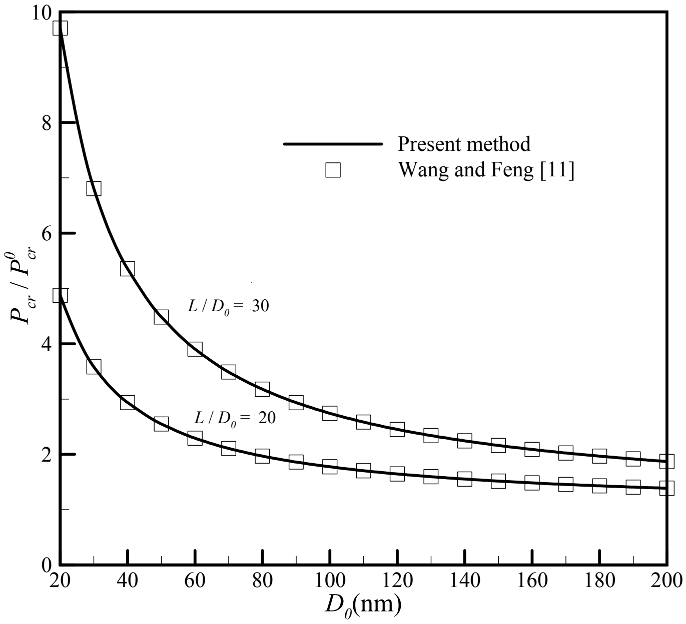

Fig. 2. The comparison of dimensionless critical buckling load of a uniform nanowire with surface effects but without nonlocal effect.

The corresponding boundary conditions are

$$Y(0)=0 \tag{8}$$

$$\frac{dY(0)}{dX}=0 \tag{9}$$

$$-E^*I^*(L)\frac{d^2Y(L)}{dX^2}+(e_0a)^2\frac{d}{dX}[(P-H(L))\frac{d^2Y(L)}{dX^2}]=0 \tag{10}$$

$$P-H(L)\frac{dY(L)}{dX}=0 \tag{11}$$

The nanowire is fixed at the end of $X=0$, then boundary conditions given by Eqs. (8) and (9) correspond to conditions of zero displacement and zero slope at $X=0$. Moreover, the Eqs. (10) and (11) correspond to zero moment and shear force at $X=L$, respectively.

The dimensionless variables are defined as follows:

$$x = X/L, \qquad y = Y/L, \qquad \alpha(x) = \frac{D(x)}{D_0}, \ \ \varepsilon = \frac{e_0 a}{L}$$

$$\xi(x) = \frac{E^* I^*(x)}{EI_0}, \ \ h(x) = \frac{H(x)L^2}{EI_0} \qquad p = \frac{PL^2}{EI_0} \tag{12}$$

where D_0 is the maximum diameter of the nonuniform nanowire at the fixed end, therefore, the flexural rigidity EI_0 of the nanowire at the fixed end should be $\pi E D_0^4/64$. Meanwhile, $\alpha(x)$, ε, $\xi(x)$, $h(x)$ and p denote the diameter ratio, dimensionless nonlocal parameter, dimensionless flexural rigidity, dimensionless residual surface tension, and dimensionless buckling load, respectively.

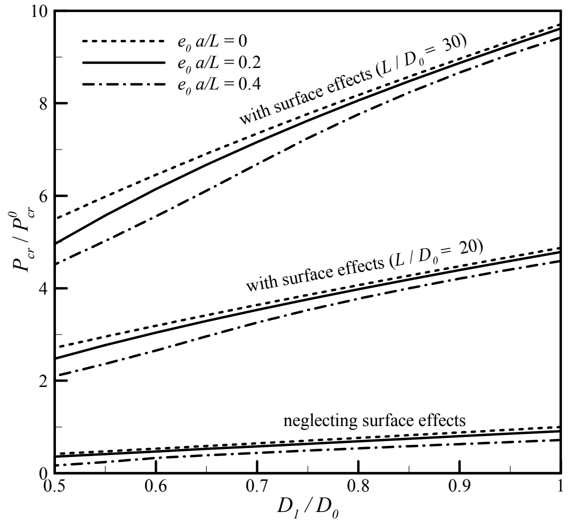

Fig. 3. The dimensionless critical buckling load of a nonuniform nanowire for different nonlocal parameters and diameter ratios.

Using the dimensionless variables given by (12), the governing equations and associated boundary conditions can be simplified to the following dimensionless forms:

$$\frac{d^2}{dx^2}[\xi(x)\frac{d^2y}{dx^2}] + (1-\varepsilon^2\frac{d^2}{dx^2})[\frac{d}{dx}(p-h(x)\frac{dy}{dx}] = 0 \tag{13}$$

$$y(0) = 0 \tag{14}$$

$$\frac{dy(0)}{dx} = 0 \tag{15}$$

$$\xi\frac{d^2y(1)}{dx^2} - \varepsilon^2\frac{d}{dx}[(p-h(1))\frac{dy(1)}{dx}] = 0 \tag{16}$$

$$(p-h(1))\frac{dy(1)}{dx} = 0 \tag{17}$$

Since the parameters $\alpha(x)$, $\xi(x)$ and $h(x)$ are dependent on the position *x* along the nanowire, the method of Rayleigh-Ritz is used to determine the critical buckling load. In order to solve Eqs.(13)-(17) by the Rayleigh–Ritz method, we set

$$y = \sum_{i=1}^{n} u_i \gamma_i(x) \tag{18}$$

where u_i are constants, and $\gamma_i(x)$ is the admissible function which required to satisfy the geometric boundary conditions, but need not satisfy the natural boundary conditions, In this present work, $\gamma_i(x) = x^{i+1}$, $i = 1,2,3,...,10$ was chosen. Then, substituting Eqs. (18) into Eqs.(13)-(17) and applying the Rayleigh quotient, the following eigenvalue problem can be obtained:

$$Ku = pMu \tag{19}$$

where *u* is the eigenvector of expansion coefficients, and

$$K_{ij} = \int_0^1 [\frac{d^2\gamma_j}{dx^2}(\xi(x)\frac{d^2\gamma_i(x)}{dx^2} + \varepsilon^2 \frac{d}{dx}(h(x)\frac{d\gamma_i(x)}{dx}) + h(x)\frac{d\gamma_j(x)}{dx}\frac{d\gamma_i(x)}{dx}]dx$$
$$-h(1)\gamma_i(1)\frac{d\gamma_i(1)}{dx} \tag{20}$$

$$M_{ij} = \int [\varepsilon^2 \frac{d^2\gamma_j(x)}{dx^2}\frac{d^2\gamma_i(x)}{dx^2} + \frac{d\gamma_j(x)}{dx}\frac{d\gamma_i(x)}{dx}]dx - \gamma_j(1)\frac{d\gamma_i(1)}{dx} \tag{21}$$

Furthermore, $\xi(x)$ and $h(x)$ given by Eq. (12) can be expressed in terms of $\alpha(x)$ as

$$\xi(x) = \alpha(x)^4 + \beta\alpha(x)^3 \tag{22}$$

$$h(x) = \gamma(\frac{L}{D_0})^2 \alpha(x) \tag{23}$$

$$\text{where } \beta = \frac{8E^S}{ED_0},\ \gamma = \frac{128\tau}{\pi E D_0}. \tag{24}$$

Solving Eq.(19) and using the dimensionless variables given by Eq. (12), the critical buckling load can be expressed as

$$P_{cr} = \frac{pEI_0}{L^2} \tag{25}$$

In case of setting $\alpha(x) = 1$ and $\varepsilon = 0$ in the above analysis, it implies that a uniform nanowire with surface effects but without nonlocal effect is assumed. For the case, the critical buckling load of a uniform nanowire can be obtained based on the analysis, and the result can also be yielded from the previous study [11]. In addition, the critical buckling load of a uniform nanowire without both surface and nonlocal effects can be written as [21]

$$P_{cr}^0 = \frac{\pi^2 EI_0}{4L^2} \tag{26}$$

3. Results and discussion

In order to compare this work with the previous study, the following surface properties are used in the analysis: $\tau = 0.89$ N□m and $E^s = 1.22$ N□m. [11] It implies the nanowire is a uniform cross-section when the value of diameter ratio D_1 / D_0 is assumed to be unity. For the different aspect ratios L / D_0, the dimensionless critical buckling load P_{cr} / P_{cr}^0 for the uniform nanowire with surface effects but without nonlocal effect is shown in Fig. 2. For the aspect ratio values of 20 and 30, it can be seen that the result excellently agrees with the previous exact result [11].

In this article, we focus on the axial buckling of a nanowire with nonuniform cross-section. The influences of surface effects, nonlocal parameter and diameter ratio on the buckling of the nonuniform nanowire are analyzed. Fig. 3 shows the dimensionless critical buckling load of a nonuniform nanowire for different nonlocal parameters and diameter ratios. The influence of surface effects on the critical buckling load is significant for different ratios. The influence becomes more and more prominent as the diameter ratio increases. The surface effects are more significant for a slender nanowire with a larger value of $\mathrm{L} / \mathrm{D}_0$. In addition, no matter whether the surface effects is considered or not, increasing the nonlocal parameter decreases the value of P_{cr} / P_{cr}^0. This is because the internal interaction force increases as the nonlocal parameter increases.

4. Conclusions

The equation for calculating the buckling load of a nonuniform nanowire with consideration of nonlocal and surface effects was analytically derived. Based on the equation, the surface and small scale effects on the buckling behavior of the nonuniform nanowire were analyzed using the Rayleigh-Ritz method. Results showed that the influence of surface effects on the critical buckling load of the nonuniform nanowire becomes more and more prominent as the diameter ratio increased. The dimensionless critical buckling load increased with increasing value of aspect ratio. When the nonlocal effect was taken into account, the critical buckling load increased with decreasing nonlocal parameter.

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