Small-size and surface effects on the axially buckling of carbon nanotubes

Yugang Sun, Xiaohu Yao[a)]

Department of Engineering Mechanics, School of Civil Engineering and Transportation,
South China University of Technology, Guangzhou, 510640, China

Summary Based on a modified nonlocal Timoshenko beam model, small-size effect and surface effect including surface elasticity and residual surface tension on the axially buckling behavior of carbon nanotubes are investigated. Explicit expression of the solution to the critical buckling load corresponding to various kinds of boundary conditions is presented. It is shown that both the small-size and surface effects have an essential impact on the critical buckling load and should be taken into account meticulously.

As basic elements of nano-electro-mechanical system (NEMS), nanobeams, carbon nanotubes (CNTs) in particular, have a leading position in the nanotechnology of precise measurement and stretchable electronics. However, with the structure size close to atom scale and the increasing ratio of surface area to volume, multiple experimental results have shown the small-size and surface effects become more and more remarkable and cannot be neglected for a better prediction of the mechanical behavior of CNTs. Consequently, the classical continuum theory must be modified in order to be applicable to the related analysis, especially the buckling stability investigation when the structure size becomes comparable to the internal scale.

Experiments on the elastic properties of nanowires were widely conducted and the composite core-shell model was proposed to predict the surface effect. Through intensive study, He and Lilley[1] farther provided a good comprehension about the surface effect including surface elasticity and residual surface tension. From the above study, the 1D linear form of the surface stress tensor is expressed as

$$\tau = \tau_0 + S\varepsilon_S \tag{1}$$

where τ_0 is the residual surface tension in the pre-buckling configuration, ε_S is the longitudinal strain of surface caused by the applied load, and $S = E_S h_S$ is the surface modulus, in which E_S and h_S are the elastic modulus and thickness of an extremely thin elastic layer covering the surface, modeling the surface elasticity, as is shown in figure 1 for the unique structure of single-walled CNTs. The influence of surface elasticity therefore can be accounted by replacing the flexural rigidity EI with the effective flexural rigidity $(EI)^*$ as follows.

$$(EI)^* = EI + E_S I_S \approx \pi E\left(d^3 t + dt^3\right)/8 + \pi S\left(d+t\right)^3/8 \tag{2}$$

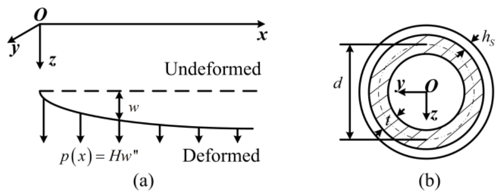

Figure 1. (a) Buckling deformation and (b) cross section of single-walled carbon nanotubes

Meanwhile, the effect of residual surface tension, the residual surface stress jump, results in a distributed transverse force $p(x)$ along the longitudinal direction according to the generalized Young-Laplace equation.

$$p(x) = H\,\partial^2 w/\partial x^2 \qquad H \approx H^0 = 2\tau_0\left(d+t\right) \tag{3}$$

On the other hand, the essence of nonlocal elasticity theory developed by Eringen[2] indicates that the stress state at a given reference point, unlike classical elasticity theory, is a function of the strain field at ever point in the body, and hence the theory could account for the influence of the long range van der Waals forces between carbon atoms and the small-size effect.

For 1D beam structure, the noted nonlocal constitutive relations in simplified differential form are written as

[a)] Corresponding author. Email: yaoxh@scut.edu.cn.

$$\sigma(x)-(e_0l_i)^2\,\partial^2\sigma(x)/\partial x^2=E\varepsilon(x)\qquad \tau(x)-(e_0l_i)^2\,\partial^2\tau(x)/\partial x^2=G\gamma(x) \tag{4}$$

where e_0 is a material constant for adjusting models in matching some reliable results, from molecular dynamics (MD) for instance. l_i is the internal characteristic length.

Following a similar procedure with the classical Timoshenko beam theory, the governing equation with consideration of surface effect in nonlocal form for the buckling behavior of axially compressed CNTs is derived as

$$\begin{cases}(EI)^*\,\partial^2\psi/\partial x^2-\kappa GA(\partial w/\partial x+\psi)=0\\ \kappa GA\left(\partial^2 w/\partial x^2+\partial\psi/\partial x\right)+\left[\left(N+H^0\right)\partial^2 w/\partial x^2-(e_0l_i)^2\left(N+H^0\right)\partial^4 w/\partial x^4\right]=0\end{cases} \tag{5}$$

The relevant nonlocal forces are obtained as

$$M=(EI)^*\,\partial\psi/\partial x-(e_0l_i)^2\left(N+H^0\right)\partial^2 w/\partial x^2\qquad Q=\kappa GA(\partial w/\partial x+\psi)-(e_0l_i)^2\left(N+H^0\right)\partial^3 w/\partial x^3 \tag{6}$$

where w and ψ are the transverse displacement and the rotation angle of the cross section, respectively; N is the axial load, G is the shear modulus, and κ is a correction factor depending on the cross section shape; M is the bending moment and Q is the shear force on the cross section.

Using boundary conditions at the two ends corresponding to different types of nanobeams, the critical buckling load for axially compressed CNTs can be solved as

$$(-N)_{Critical}=\frac{(\pi/\eta L)^2\,(EI)^*}{1+\left[(EI)^*/\kappa GA+(e_0l_i)^2\right](\pi/\eta L)^2}+H^0 \tag{7}$$

Related to different boundary conditions, the coefficient η herein still takes the same value as that given in classical Euler-Bernoulli beam theory for the three representative beams, that is, $\eta=1$ for simply supported beams, $\eta=2$ for fixed-free beams, and $\eta=0.5$ for fixed-fixed beams. A glimpse at figure 2 presented below reveals the distribution of the critical buckling load with respect to related parameters. It is demonstrated that small-size and surface effects obviously make the results of the modified Timoshenko beam model closer to those of MD simulations. Besides, influence of the nonlocal parameter e_0 is contrary to that of the surface properties (S and τ_0).

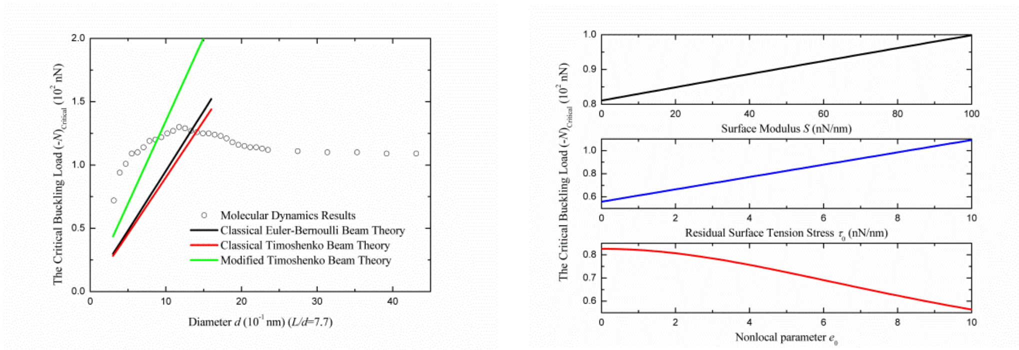

Figure 2. Distribution of the critical buckling load for representative single-walled carbon nanotubes changing with (a) diameter, (b) the nonlocal parameter, the surface modulus, and the residual surface tension

By way of conclusion, the small-size and surface effects are taken into consideration synchronously in the axial buckling analysis of CNTs based on a modified Timoshenko beam model and analytic solution to the critical buckling load corresponding to different kinds of boundary conditions is presented for the first time. It is evident that both the small-size effect and surface effect have an essential impact on the buckling stability of CNTs.

References

[1] He J., Lilley C.M.: Surface Effect on the Elastic Behavior of Static Bending Nanowires. *Nano Lett.* **8**:1798-1802, 2008.

[2] Eringen A.C.: On Differential Equations of Nonlocal Elasticity and Solutions of Screw Dislocation and Surface Waves. *J. Appl Phys* **54**:4703-4710, 1983.