Bending analysis of carbon nanotubes using nonlocal continuum models

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Abstract. Experiments show that a CNT can withstand large bending curvature reversibly. As the deflection is severe for large varying forces, the elementary elastic theory cannot be applied. Again, the classical (or local) continuum elastic theory is questionable at very small length scale (less than 100 nm) because the material microstructure, such as lattice spacing between individual atoms, become important. For studying mechanical properties of carbon nanotubes (CNTs) of small length, the classical theory can be modified by using nonlocal continuum models proposed by Eringen. In the present work, static analysis of CNT is presented using a nonlinear relation between the bending curvature and the beam deflection and the nonlocal continuum mechanics models. It is shown that there is an upper bound on the load on a cantilevered CNT.

Keywords: Nonlocal continuum models, carbon nanotubes, static analysis, upper bound.

1. Introduction
Both experimental and theoretical studies show that CNTs exhibit superior mechanical, electronic, electrochemical and thermal properties over many known materials. Many experiments have been performed to study their mechanical properties like strength, stiffness etc. which can be inferred from measuring the values of tensile strength ($\sigma_s$) and Young’s modulus ($E$) respectively. Experimental measurements of mechanical property of CNTs involve the techniques such as transmission electron microscope (TEM), scanning electron microscope (SEM) and atomic force microscope (AFM). From experiments it is found that CNTs have high tensile strength ($\sim 150$ GPa) and Young’s modulus ($\sim 1$ TPa) in addition to small size ($\sim$ nm) and low weight ($\sim$ one-sixth of steel). Because of these properties they present a promising nanoscale material for building different kinds of nanodevices in nanoelectromechanical systems (NEMS) and many other applications. Most potential applications of CNTs are heavily based on a thorough understanding of their mechanical behaviours. However, their mechanical properties have not fully predicted. A detail study of the mechanical properties of CNTs will be important for such applications. Most estimates of $E$ have been obtained by using elementary elastic theory.

In order to determine the effective value of $E$ of multiwalled carbon nanotubes (MWCNTs), in an experiment, Wong et al. [1] applied an external force at different locations along a cantilevered MWCNT and measured deflection versus bending force using AFM. They observed that the CNT show remarkable flexibility and large elastic deformation without breaking. And also they noted that the strain energy increases quadratically with deflection as expected for a harmonic system, whereas for large deflection the strain energy showed a deviation from the usual harmonic behaviour. Some more experiments have also shown that CNTs can withstand large bending curvatures reversibly [2-3]. The linear theory, which is valid only for small bending deformations, cannot explain such behaviour. However, the above behaviour can be explained by considering the nonlinear relation between the bending curvature $K(x)$ and the beam deflection $\omega(x)$ [4].
Carbon nanotubes are of nanometer size and the experimental error is quite high due to lack of information about its diameter and thickness of layers. Further, conducting experiments with such types of specimens are difficult and costly. Hence it is essential to develop an appropriate mathematical model to study its mechanical properties, which is the subject of recent research in computational nanomechanics and computational condensed matter physics. Two approaches are widely used for the theoretical study on CNTs: molecular dynamics simulation and continuum mechanics methods. However, the former one is very time-consuming and remains formidable for large-scale systems. Hence we will follow the latter in which CNTs are modelled as elastic beams such as Timoshenko, Euler-Bernoulli, shells and elastic rods, which have been widely and successfully used to study the mechanical behaviour of nanostructures such as CNTs, graphene sheets, nanofibres etc. Again, the classical continuum elastic theory, which is quite reliable for mechanical properties of CNTs of length scales 100 nm and more [5], is questionable at very small length scale (less than 100 nm) [6] because the material microstructure, such as lattice spacing between individual atoms, become important. This suggests that the classical theory needs to be modified. This was formally done by Eringen’s nonlocal continuum models [7] which extend the continuum approach to smaller length scale.

In the present work, we have used nonlocal constitutive equations of Eringen [8] and the nonlinear relation between the bending curvature $K(x)$ and the beam deflection $\omega(x)$ to obtain analytic solution for large deflection for a cantilevered CNT. We have found that there is an upper bound on the load that can be applied at the tip of the free end of a cantilevered CNT which can be regarded as the maximum load needed for breaking the tube.

2. Fundamental aspects of non-local continuum models
The classical continuum models assume that the stress at a given point $x$ in a body is dependent uniquely on the strain state at that same point in the body. Hence the models are usually called local continuum models and local elasticity is inherently size-independent. The constitutive equation of classical elasticity, an algebraic relationship between the stress and strain, is given by

$$\sigma(x) = E \varepsilon(x),$$

where $\sigma(x)$ and $\varepsilon(x)$ are the stress and the strain respectively. However, at nanometer scales the microstructure of the material, such as the lattice spacing between individual atoms, becomes increasingly important and the discrete structure of the material can no longer be homogenized into a continuum. The nonlocal elasticity models of Eringen [7] abandon the classical assumption of locality and assume that the stress at any reference point in the body depends not only on the strains at that point but also on the strains of at all points of the body. This is based on the atomic theory of lattice dynamics and some experimental observations on phonon dispersion. If the effects of strains at points other than the reference point are ignored, one obtains local continuum model. Thus in nonlocal continuum mechanics, the long range forces between atoms and the internal scale effect are considered in construction of constitutive equations. The most general form of the constitutive equation for nonlocal elasticity involves an integral over the entire region of interest. This integral contains a kernel function which describes the relative influences of strains at various locations on the stress at a given location.

For homogeneous and isotropic elastic solids, the nonlocal stress tensor at point $x$ is given by

$$\sigma_{ij}(x) = \int_V \alpha(|x' - x|, \tau) \sigma_{ij}^{(c)}(x') \, dV(x') \quad \text{for } x \in V,$$
where $\sigma_{ij}(x')$ is the classical, macroscopic stress tensor at point $x'$, and is equal to $C_{ijkl} \varepsilon_{kl}(x)$ ($C_{ijkl}$ = the elastic modulus tensor of classical isotropic elasticity and $\varepsilon_{kl}(x)$ = the strain tensor). $\alpha(|x' - x|, \tau)$ is the nonlocal modulus (or the kernel function), which incorporates the nonlocal effect at the reference point $x$ produced by local strain at the source $x'$ into the constitutive equations. Here $|x' - x|$ is the Euclidean distance and the material constant $\tau$ is given by $\tau = e_0 \alpha/\ell$ [9].

For CNT, the value of $e_0$ has not been determined by experiment. The value of the adjustable parameter $e_0$ has been taken as 0.39 by Eringen [8], whereas Sudak has proposed its value in the order of hundreds [5]. Further, the value of parameter ‘$\alpha$’ can be chosen to be the distance between C – C bonds which is equal to 0.142 nm [5]. For carbon nanotubes in one-dimensional case, equation (3) becomes

$$\left(1 - (e_0 \alpha)^2 \nabla^2\right) \sigma_{ij}(x) = \sigma_{ij}(x'),$$

where $\nabla^2$ denotes the second order spatial gradient (the Laplacian). The characteristic length $e_0 \alpha$ account for the so-called nonlocal effects. For CNT, the value of $e_0$ has not been determined by experiment. The value of the adjustable parameter $e_0$ has been taken as 0.39 by Eringen [8], whereas Sudak has proposed its value in the order of hundreds [5]. Further, the value of parameter ‘$\alpha$’ can be chosen to be the distance between C – C bonds which is equal to 0.142 nm [5]. For carbon nanotubes in one-dimensional case, equation (3) becomes

$$\left(1 - (e_0 \alpha)^2 \frac{d^2}{dx^2}\right) \sigma(x) = E \varepsilon(x).$$

### 3. General method of determining nonlocal equations of bending of carbon nanotubes

Consider an infinitesimal element PQRS of length $dx$ of a beam under uniformly distribution load $p$. Let $V$ and $V + dV$ be the shear forces at the left and the right faces of the element during its downward displacement. And the corresponding internal resisting moment at the left face due to the left portion of the beam is $M$ in the clockwise direction and at the right portion of the beam is $M + dM$ in the counter clockwise direction. The free body diagram of the beam element is shown in figure 1.

![Figure1](image.png)

**Figure1.** An infinitesimal element under uniformly distributed load.

The element must be equilibrium under the action of these forces and couples. The equilibrium equation for the vertical force component is

$$V - pdx - (V + dV) = 0.$$
This gives

$$p(x) = -\frac{dV(x)}{dx}.$$  \hspace{3cm} (5)$$

Taking moments about C, the moment equilibrium equation is written as

$$M + V \times \left(\frac{1}{2} dx\right) + (V + dV) \times \left(\frac{1}{2} dx\right) - (M + dM) = 0.$$  

Neglecting the product of the infinitesimally small quantities $dV \times dx$, we obtain

$$V(x) = \frac{dM(x)}{dx}.$$  \hspace{3cm} (6)$$

Substituting this into equation (5), we obtain

$$p(x) = -\frac{d^2M(x)}{dx^2}.$$  \hspace{3cm} (7)$$

From definitions, the bending moment $M$ and the axial strain $\epsilon(x)$ for large deflection of the CNT are given by [11]

$$M(x) = \int_A \sigma(x)y \, dA \quad \text{and} \quad \epsilon(x) = -yK(x),$$  \hspace{3cm} (8)$$

where $y$ is the coordinate measured from the mid-plane in the height direction of the beam, $A$ the area of the cross-section of the beam. The curvature $K(x)$ is related to the vertical deflection $\omega(x)$ of CNT at $x$ by [12]

$$K(x) = \frac{\omega''(x)}{\left[1 + [\omega'(x)]^2\right]^{3/2}},$$  \hspace{3cm} (9)$$

where $(\cdot')$ denotes differentiation with respect to $x$. Now the Euler-Bernoulli relation between strain and curvature becomes

$$\epsilon(x) = -\frac{y\omega''(x)}{\left[1 + [\omega'(x)]^2\right]^{3/2}}.$$  \hspace{3cm} (10)$$

Combining equations (4) and (10), we have

$$\left[1 - (\epsilon_0a)^2 \frac{d^2}{dx^2}\right] \sigma(x) = -\frac{Ey\omega''(x)}{\left[1 + [\omega'(x)]^2\right]^{3/2}}.$$  \hspace{3cm} (11)$$

Multiplying both sides of equation (11) by $y$ and integrating over $A$, we obtain

$$\int_A \sigma(x)y \, dA - \int_A (\epsilon_0a)^2 \frac{d^2\sigma(x)}{dx^2} y \, dA = \int_A -\frac{Ey\omega''(x)}{\left[1 + [\omega'(x)]^2\right]^{3/2}} y \, dA.$$  

By using the definition of bending moment the above equation becomes

$$M(x) - (\epsilon_0a)^2 \frac{d^2M(x)}{dx^2} + EI \frac{\omega''(x)}{\left[1 + [\omega'(x)]^2\right]^{3/2}} = 0,$$

where $I = \int_A y^2 \, dA$ is the moment of inertia and $EI$ is the bending rigidity of the beam structure. Using equation (7), the expression for the nonlocal bending moment is given by
\begin{equation}
M(x) = -(e_0 a)^2 p(x) - EI \frac{\omega''(x)}{(1 + [\omega'(x)]^2)^{3/2}}.
\end{equation}

Using equation (6) the nonlocal shear force \( V(x) \) can be expressed as

\begin{equation}
V(x) = -(e_0 a)^2 \frac{d^2 p(x)}{dx^2} - EI \frac{d^2}{dx^2} \left[ \frac{\omega''(x)}{(1 + [\omega'(x)]^2)^{3/2}} \right].
\end{equation}

From equation (5), we have

\[ p(x) = -\frac{dV(x)}{dx} = (e_0 a)^2 \frac{d^2 p}{dx^2} + EI \frac{d^2}{dx^2} \left[ \frac{\omega''(x)}{(1 + [\omega'(x)]^2)^{3/2}} \right]. \]

Or,

\begin{equation}
EI \frac{d^2}{dx^2} \left[ \frac{\omega''(x)}{(1 + [\omega'(x)]^2)^{3/2}} \right] - \left[ 1 - (e_0 a)^2 \frac{d^2}{dx^2} \right] p(x) = 0.
\end{equation}

This is the Euler-Bernoulli beam equation for nonlocal beam model for CNTs subjected to a distributed load. When \( e_0 = 0 \), the above equation reduces to

\begin{equation}
EI \frac{d^2}{dx^2} \left[ \frac{\omega''(x)}{(1 + [\omega'(x)]^2)^{3/2}} \right] - p(x) = 0,
\end{equation}

which is the local Euler-Bernoulli beam equation for large deflection. Again, for small deflection the slope \( \omega'(x) \) is small, we can neglect \([\omega'(x)]^2\) in comparison with 1 in equation (14) and obtain the following equation for nonlocal case

\begin{equation}
EI \frac{d^4 \omega(x)}{dx^4} - \left[ 1 - (e_0 a)^2 \frac{d^2}{dx^2} \right] p(x) = 0.
\end{equation}

And the local Euler-Bernoulli beam equation for small deflection becomes

\begin{equation}
EI \frac{d^4 \omega(x)}{dx^4} - p(x) = 0.
\end{equation}

As a simple example, we study small-scale effects on the response of a cantilevered CNT of length \( L \) clamped at \( x = 0 \) and free at the other end used as an actuator. When a concentrated force \( P(x) \) is applied at \( x \) on the beam the governing equation (14) gives

\begin{equation}
EI \frac{d^2}{dx^2} \left[ \frac{\omega''(x)}{(1 + [\omega'(x)]^2)^{3/2}} \right] - \left[ 1 - (e_0 a)^2 \frac{d^2}{dx^2} \right] P(x) = 0.
\end{equation}

The load applied at \( x = l \ (l < L) \) can be written as \( P(x) = P \delta(x - l) \), where \( \delta \) is the Dirac delta function. Then equation (18) becomes

\begin{equation}
EI \frac{d^2}{dx^2} \left[ \frac{\omega''(x)}{(1 + [\omega'(x)]^2)^{3/2}} \right] = P \left[ 1 - (e_0 a)^2 \frac{d^2}{dx^2} \right] \delta(x - l).
\end{equation}

Integrating the above equation we have

\begin{equation}
EI \frac{d}{dx} \left[ \frac{\omega''(x)}{(1 + [\omega'(x)]^2)^{3/2}} \right] = P[H(x - l) - (e_0 a)^2 \delta'(x - l)] + C_1,
\end{equation}

\( H \) is the Heaviside step function.
where the Heaviside function \( H(x - l) = \int \delta(x - l)dx \) and \( C_1 \) is a constant of integration. Integrating equation (19) again we have

\[
EI \left[ \frac{\omega''(x)}{[1+\omega'(x)^2]^{3/2}} \right] = P\left[x-l\right]H(x-l) - (e_0a)^2\delta(x-l) + C_1x + C_2.
\]  

(20)

This is a non-linear differential equation governing \( \omega(x) \). Putting \( u(x) = \omega'(x) \), the above equation becomes

\[
d\frac{u(x)}{[1+[u(x)]^2]^{3/2}} = \frac{1}{EI} \{ P\left[x-l\right]H(x-l) - (e_0a)^2H(x-l) \} + C_1 \frac{x^2}{2} + C_2x + C_3.
\]

On further integration we obtain

\[
\frac{\omega'(x)}{[1+\omega'(x)^2]^{1/2}} = \frac{1}{EI} \left\{ P\left[\frac{(x-l)^2}{2}\right]H(x-l) - (e_0a)^2H(x-l) \right\} + C_1 \frac{x^2}{2} + C_2x + C_3 \equiv f(x) .
\]

(21)

On squaring equation (21) becomes

\[
\frac{[\omega'(x)]^2}{[1+\omega'(x)^2]^2} = [f(x)]^2.
\]

Simplifying the above equation we obtain

\[
\omega(x) = \int \frac{f(x)}{[1+[f(x)]^2]^{1/2}} dx + C_4,
\]

(22)

where \( C_4 \) is the constant of integration. All the constants of integrations \( C_i \) \((i=1,2,3,4)\) can be determined from the boundary conditions. For the cantilevered beam, the boundary conditions are

\[
\omega(x) |_{x=0} = \omega'(x) |_{x=0} = 0 \quad \text{and} \quad M(x) |_{x=L} = V(x) |_{x=L} = 0.
\]

(23)

The first boundary conditions give \( C_3 = C_4 = 0 \) and the second boundary conditions give \( C_1 = -P \) and \( C_2 = PL \). Thus equation (23) becomes

\[
\omega(x) = \int \frac{g(x)}{[1+[g(x)]^2]^{1/2}} dx
\]

where

\[
g(x) = \frac{P}{EI} \left\{ \left[ \frac{(x-l)^2}{2}H(x-l) - (e_0a)^2H(x-l) \right] - \frac{x^2}{2} + Lx \right\}.
\]

(24)

This is the expression of total deflection in nonlocal models for a cantilevered CNT. Equation (24) shows that the small scale term vanishes in the domain \( x < l \), but it will affect when \( x > l \).

3.1. Expression for upper bound on the load

The value of total deflection of the bent CNT in equation (24) should be real. This puts a restriction on the value of the denominator. This gives

\[
[g(x)]^2 < 1.
\]
Taking the square root we obtain

\[ g(x) = \frac{P}{EI} \left\{ \left[ \frac{(x-l)^2}{2} - (e_0a)^2 H(x - l) \right] - \frac{x^2}{2} + Lx \right\} < 1. \]  \hspace{1cm} (25)

For the load at the tip of the free end of the CNT, \( x = L \). This gives

\[ P_{\text{max}} < \frac{2EI}{l^2 - (e_0a)^2}. \]  \hspace{1cm} (26)

This is the expression of upper bound on the load in nonlocal models that can be applied at the tip of the free end of a cantilevered CNT which can be regarded as the maximum load needed for breaking the tube. It is evident that the small-scale term has an effect on the value of the maximum load for CNTs having small length (less than 100 nm). When \( e_0 = 0 \), the above equation reduces to

\[ P_{\text{max}} < \frac{2EI}{L^2}. \]  \hspace{1cm} (27)

This gives the maximum load needed for breaking the CNT which depends on the rigidity \( EI \) and on the length \( L \) of the CNT as is the case in classical theory.

4. Conclusions

By using the nonlocal Euler-Bernoulli beam theory, we have derived analytical expressions for large deflection for a cantilevered CNT. It is found that there is an upper bound on the load that can be applied at the tip of the free end of a cantilevered CNT which can be regarded as the maximum load needed for breaking the tube. Our results can be used for studying nanoelectromechanical cantilevered systems of small length scale.

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