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Bernoulli-Euler beam theory of single-walled carbon nanotubes based on nonlinear stress-strain relationship

Kun Huang\textsuperscript{1,2,*}, Xiping Cai\textsuperscript{1} and Mingguang Wang\textsuperscript{1}

\textsuperscript{1} Department of Engineering Mechanics, Faculty of Civil Engineering and Mechanics, Kunming University of Science and Technology, Kunming 650500, People’s Republic of China

\textsuperscript{2} Yunnan Key Laboratory of Disaster Reduction in Civil Engineering, Kunming University of Science and Technology, Kunming 650500, People’s Republic of China

E-mail: kunhuang2008@163.com

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Abstract

Recent experiments and density functional tight-binding (DFTB) calculations indicated the nonlinear elastic properties of graphene. However, this nonlinear stress-strain relationship has not been applied to the carbon nanotubes (CNTs) that can be viewed as graphene sheets that have been rolled tubes. In this paper, using the nonlinear stress-strain relationship of graphene, a new Bernoulli-Euler beam model of single-walled carbon nanotubes (SWCNTs) is presented for the first time. The static bending and the first-order mode forced vibrations of SWCNTs are investigated according to the new model. The results indicate that the nonlinear stress-strain relationship has a significant influence on the mechanical properties of SWCNTs.

1. Introduction

Some of the most important potential applications of nanostructures are related to their mechanical properties [1–4], but to model the nanostructures’ mechanical properties accurately is difficult. Although the classical elasticity theory is usually used to model nanostructures in practice, many questions still need to study thoroughly. For example, solid-solid interfaces may play a crucial role in mechanical properties of nanostructures because the interfaces generate additional surface stress due to elastic deformations [5, 6]. When the phase transitions between austenite to martensitic variants and twinning between martensitic variants, a phase field approach can capture the effects of interfacial stress on phase transformations for NiAl shape memory alloys [7–9]. So far, the mechanical properties of CNTs have been mainly studied through experiments, molecular dynamics (MD) simulations, DFTB calculations [1, 2]. MD and DFTB approaches require huge computational resources and are limited to simulating about $10^6$ atoms for a few nanoseconds. For this reason, the macroscopic continuum mechanics techniques are becoming increasingly popular. Chemically, the $sp^2$-hybridized covalent bonds of carbons mainly form the $\sigma$ skeleton of the honeycomb lattice. The skeleton can be modeled as a film, and only two independent in-plane elastic constants are needed to characterize the film’s mechanical properties due to the hexagonal symmetry of the structure. The two-dimensional (2D) Young’s modulus and Poisson’s ratio are commonly used in practice, in which they have been extensively discussed [1, 2, 10]. The stiff $\sigma$-bonds give graphene an exceptionally high 2D Young’s modulus. Although the interrelation between atomistic reason and continuum material descriptions is still not very well established, the continuum mechanics can still obtain results consistent with experiments, MD, and DFTB calculations [10–13].

A distinct characteristic of nanomechanics is that the mechanical properties of nanomaterials are size-dependent. So some researchers believe that the nonlocal (or couple stress) effect may be considered when the classical macroscopic continuum mechanics is applied to nanostructures [14–17]. However, for the mechanical properties of SWCNTs with large diameters ($>$1 nm), the theoretical calculations show that the size-dependent effect may be ignored [14, 15]. Recently, DFTB calculations and experiments have shown that the stress-strain relationship of graphene is nonlinear [18–20]. The nonlinear stress-strain relationship has a significant impact...
on graphene’s mechanical properties [21–23]. From the existing quantum calculations, it has also been found that the stress-strain relationships of many single-layer 2D structures are nonlinear, such as BN [24], graphyne [25], etc. However, the effects of nonlinear stress-strain relations on their mechanical properties have not been intensively studied. For SWCNTs, the experiments and theoretical calculations of nonlinear constitutive relation have been reported barely. SWCNTs can be viewed as a graphene sheet that has been rolled into a tube, so the graphene’s stress-strain relationship may be consistent with that of SWCNTs. So far, the nonlinear constitutive relation has not been applied to SWCNTs, and researchers have not yet paid attention to its effects on mechanical properties. In this paper, the nonlinear stress-strain relationship will be used to establish the Bernoulli-Euler beam model of SWCNTs.

2. Theoretical formulation

By measuring the uniaxial strain and stress of graphene, Lee et al [18] obtained a nonlinear stress-strain relationship of graphene using an atomic force microscope. Later, three second-order and four third-order elastic constants of graphene were obtained by the DFTB calculations [19, 20]. Recent atomic calculations have also shown that other monolayer carbon materials’ stress-strain relationships are also nonlinear [25]. For simplicity, only the first- and second-order elastic constants of graphene are considered in the present research. As shown below, the quadratic nonlinear term of the stress-strain relationship adds a few cubic nonlinear terms to the beam model of SWCNTs. For the classical Bernoulli-Euler beam, as shown in figure 1, only the longitudinal stress is considered, and the beam’s nonlinear stress-strain relationship is written as [18]

\[
\sigma_{xx} = Ee_{xx} + De_{xx}^2,
\]

where \(\sigma_{xx}\) and \(e_{xx}\) are stress and strain in the x-axis direction. The experiments showed \(E = 1.0TPa\) and \(D = -2.0TPa\) for graphene [18]. Suppose \(u\) and \(w\) are displacements of the beam axis in the x and y direction respectively, as shown in figure 1, the equations of motion of the Bernoulli-Euler beam are [26]

\[
\begin{align*}
\partial N / \partial x &= m \partial^2 u / \partial t^2, \\
\partial^2 M / \partial x^2 + N \partial^2 w / \partial x^2 &= m \partial^2 w / \partial t^2 + F(x, t),
\end{align*}
\]

where \(N\) and \(M\) are the axial force and the bending moment of the cross-section; \(m\) is mass per unit length; \(F(x, t)\) is the load in the y-direction, and the load in the x-direction is neglected. Using equation (1), gives

\[
N = \int_A \sigma_{xx} dA = \int_A \int_A (Ee_{xx} + De_{xx}^2) dA,
\]

\[
M = \int_A y e_{xx} dA = \int_A \int_A y(Ee_{xx} + D e_{xx}^2) dA.
\]

Here \(A\) is the cross-section area. The Green strain tensor is used in general, but the terms containing \(\gamma^2\) may be neglected in view of the beam’s slenderness. So the Von Karman strain [26, 27] is used in this paper, as

\[
\varepsilon_{xx} = \frac{\partial u}{\partial x} - y \frac{\partial^2 w}{\partial x^2} + \frac{1}{2} \left( \frac{\partial w}{\partial x} \right)^2.
\]

In equation (4), we assume \(\partial u / \partial x\) is roughly equal to \((\partial w / \partial x)^2\) because the square of the slope and the strain of the centroid locus are small compared to unity. Substitute equation (4) into equation (3), gives

![Figure 1. Schematic diagram of (a) a beam under a distributed lateral load and (b) a cross-section.](image-url)
\[
N = ID \left( \frac{\partial^2 w}{\partial x^2} \right)^2 + EA \left[ \frac{\partial u}{\partial x} + \frac{1}{2} \left( \frac{\partial w}{\partial x} \right)^2 \right] + DA \left[ \frac{\partial u}{\partial x} + \frac{1}{2} \left( \frac{\partial w}{\partial x} \right)^2 \right]^2,
\]

\[
M = -EI \frac{\partial^2 w}{\partial x^2} - 2ID \left[ \frac{\partial u}{\partial x} + \frac{1}{2} \left( \frac{\partial w}{\partial x} \right)^2 \right] \frac{\partial^4 w}{\partial x^4},
\]

where \( I = \int_A y^2 dA \) is the second moment of area of the cross-section. Substituting \( N \) and \( M \) into equation (2), gives

\[
-\left[ \frac{\partial u}{\partial x} + \frac{1}{2} \left( \frac{\partial w}{\partial x} \right)^2 \right] \frac{\partial^2 w}{\partial x^2} - 2ID \left[ \frac{\partial u}{\partial x} + \frac{1}{2} \left( \frac{\partial w}{\partial x} \right)^2 \right] \frac{\partial^4 w}{\partial x^4} - DA \left[ \frac{\partial u}{\partial x} + \frac{1}{2} \left( \frac{\partial w}{\partial x} \right)^2 \right]^2
\]

\[
+ \left[ \frac{\partial u}{\partial x} + \frac{1}{2} \left( \frac{\partial w}{\partial x} \right)^2 \right] \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 u}{\partial x^2} \left( \frac{\partial^2 w}{\partial x^2} \right)^2
\]

\[
+ 3 \frac{\partial^2 w}{\partial x^2} \frac{\partial^3 w}{\partial x^3} + \frac{1}{2} \frac{\partial^3 w}{\partial x^3} \frac{\partial^4 w}{\partial x^4}
\]

\[
- \frac{\partial^2 w}{\partial x^2} \left[ EA \left[ \frac{\partial u}{\partial x} + \frac{1}{2} \left( \frac{\partial w}{\partial x} \right)^2 \right]^2
\]

\[
+ DA \left[ \frac{\partial u}{\partial x} + \frac{1}{2} \left( \frac{\partial w}{\partial x} \right)^2 \right]^2 + ID\left( \frac{\partial^2 w}{\partial x^2} \right)^2 \right]\}
\]

\[
= m \frac{\partial^2 w}{\partial t^2} + F(x, t).
\]

For a hinged-hinged beam, the boundary conditions are

\[
u = w = \frac{\partial w}{\partial x} = 0 \text{ at } x = 0 \text{ and } l
\]

The inertia term in equation (6) may be omitted for slender beams, and \( u \) is mainly induced by the transverse deformation \( w \) \cite{26}. So equation (6) can be simplified as follows:

\[
\frac{\partial^2 u}{\partial x^2} = -\frac{\partial w}{\partial x} \frac{\partial^2 w}{\partial x^2} - 2\lambda \frac{\partial^2 w}{\partial x^2} \frac{\partial^4 w}{\partial x^4},
\]

where \( \lambda = ID / EA \). Integrating (9) twice with respect to \( x \), we get

\[
\frac{\partial u}{\partial x} = -\frac{1}{2} \left( \frac{\partial w}{\partial x} \right)^2 - \lambda \left( \frac{\partial^2 w}{\partial x^2} \right)^2 + c_0(t),
\]

\[
u = -\frac{1}{2} \int_0^x \left( \frac{\partial w}{\partial s} \right)^2 + 2\lambda \left( \frac{\partial^2 w}{\partial s^2} \right)^2 ds
\]

\[+ c_0(t)x + c_2(t).
\]

The second formula in equation (10) is the integral with the changing upper limit of the first formula. Imposing the boundary conditions (8) yields \( c_2(t) = 0 \) and

\[
c_0(t) = \frac{1}{2\lambda} \int_0^l \left[ \left( \frac{\partial w}{\partial s} \right) \frac{\partial^2 w}{\partial s^2} \right]^2 ds.
\]

Differentiating equation (9) once with respect to \( x \), we have

\[
\frac{\partial^2 u}{\partial x^2} = -\left( \frac{\partial^2 w}{\partial x^2} \right)^2 - \frac{\partial w}{\partial x} \frac{\partial^4 w}{\partial x^4} - 2\lambda \frac{\partial^2 w}{\partial x^2} \frac{\partial^4 w}{\partial x^4} - 2\lambda \frac{\partial^2 w}{\partial x^2} \frac{\partial^4 w}{\partial x^4}.
\]
Substituting \( \partial^4 u / \partial x^2 \), \( \partial^2 u / \partial x^2 \) and \( \partial u / \partial x \) into equation (7), and keeping up to the cubic terms in \( w \), gives

\[
m \frac{\partial^4 w}{\partial t^2} + C \frac{\partial w}{\partial t} + EI \frac{\partial^4 w}{\partial x^4} - EA \left( \frac{\partial^2 w}{\partial x^2} - 2 \lambda \frac{\partial^2 w}{\partial x^4} \right)
- 6ID \lambda \left[ \frac{\partial^2 w}{\partial x^2} \left( \frac{\partial^2 w}{\partial x^3} \right)^2 \right] = F(x, t).
\]

Here it is assumed that the damping is proportional to the velocity, i.e. damping term \( C (\partial w / \partial t) \) is added in equation (12). For simplification, we suppose the load is a simple harmonic function in time, i.e. \( F(x, t) = f(x) \cos \omega t \). Equation (12) may be written in a dimensionless form by defining the quantities

\[ \pi = x/l, \quad I = \omega_0 t, \quad \omega = w/l. \]

Here \( \omega_0 = \sqrt{\pi^4 EI/l^4 m} \) is the natural frequency of a hinged–hinged beam. So equation (12) can be rewritten as

\[
\frac{\partial^2 w}{\partial \pi^2} + \frac{C}{m \omega_0} \frac{\partial w}{\partial \pi} + \frac{4 \pi^2}{\pi^4} \left( \frac{\partial^2 w}{\partial \pi^2} \right)^2 \left( \frac{\partial^2 w}{\partial \pi^2} \right)^2
- 6ID \lambda \frac{\partial^2 w}{\partial \pi^2} \left( \frac{\partial^2 w}{\partial \pi^2} \right)^2 \left( \frac{\partial^2 w}{\partial \pi^4} \right)
- \frac{EA}{2 m \omega_0^2 l^2} \left( \frac{\partial^2 w}{\partial \pi^2} - \lambda \frac{\partial^4 w}{\partial \pi^4} \right) \int_0^1 \left( \frac{\partial^2 w}{\partial \pi} \right)^2 \, d\pi
+ \frac{2 \lambda}{l^2} \left( \frac{\partial^2 w}{\partial \pi^2} \right)^2 \, dx = \frac{f(\pi)}{ml \omega_0^2} \cos \omega \pi, \tag{13}
\]

here \( \omega = \omega_0 / \omega_0 \). For slender tubes, has \( \lambda/l^2 \ll 1 \), as a result, the nonlinear terms of \( \lambda/l^6 \) may be discarded, gives

\[
\frac{\partial^2 \dot{w}}{\partial \pi^2} + \frac{C}{m \omega_0} \frac{\partial \dot{w}}{\partial \pi} + \frac{4 \pi^2}{\pi^4} \left( \frac{\partial^2 \dot{w}}{\partial \pi^2} \right)^2 \left( \frac{\partial^2 \dot{w}}{\partial \pi^2} \right)^2
- \frac{EA}{2 m \omega_0^2 l^2} \left( \frac{\partial^2 \dot{w}}{\partial \pi^2} - \lambda \frac{\partial^4 \dot{w}}{\partial \pi^4} \right) \int_0^1 \left( \frac{\partial^2 \dot{w}}{\partial \pi} \right)^2 \, d\pi
+ \frac{ID}{m \omega_0^2 l^2} \frac{\partial^4 \dot{w}}{\partial \pi^4} \int_0^1 \left( \frac{\partial^2 \dot{w}}{\partial \pi} \right)^2 \, dx = \frac{f(\pi)}{ml \omega_0^2} \cos \omega \pi. \tag{14}
\]

3. Static bending and forced vibration analysis

Equation (14) is a nonlinear partial differential integral equation, and it is difficult to obtain an exact analytical solution. So the Galerkin method is used to find an approximate solution of the equation. Suppose equation (14) has a solution

\[ w = \sum_{n=1}^{\infty} \eta_n(\pi) \sin(n\pi \pi), \]

and only the first term is used for simplicity, and let \( \eta_0 = \eta \). Substituting equation (15) into equation (14), multiplying by \( \sin \pi \pi \), and integrating over the interval [0, 1](the Galerkin procedure), gives

\[
\frac{\partial^2 \eta}{\partial \pi^2} + \frac{C}{m \omega_0} \frac{\partial \eta}{\partial \pi} + k_1^2 \eta + k_3 \eta = \tilde{f} \cos \omega \pi, \tag{16}
\]

where \( k_1^2 = \frac{\beta n_{\pi}(\pi)}{m \omega_0}, \quad k_3 = \frac{E A \pi^4}{m \omega_0 l^2} \left( 1 + \frac{4 \pi^2}{l^2} \right), \quad \tilde{f} = \frac{C}{m \omega_0} \) and \( \tilde{f} = \frac{2 \lambda}{ml \omega_0^2} \int_0^1 f(\pi) \sin\pi \pi \, d\pi \). In fact, neglects the inertia and damping terms, the algebraic equation to determine the amplitudes of static bending is

\[
\tilde{k}_1 \eta + \tilde{k}_3 \eta = \tilde{f}. \tag{17}
\]

From equation (17), the static mid-point deformations of SWVNTs can be obtained. Figure 2 shows the relationship between the deformations and loads for a (15, 15) armchair SWCNT.
In order to research the dynamic behaviors, we perturb equation (16). Let \( \tilde{\varepsilon} = 2\varepsilon^2\varepsilon \) and \( \tilde{\varepsilon}^2 = f \). \( \varepsilon \) is a small parameter and \( \varepsilon = 0.1 \) is used in this paper, consequently equation (16) can be rewritten as

\[
\frac{\partial^2 \eta}{\partial t^2} + k_1^2 \eta + 2\varepsilon^2\varepsilon \frac{\partial \eta}{\partial t} + k_3 \eta^3 = \varepsilon^3 f \cos \omega t.
\]  

(18)

Here the method of multiple scales is used to solve equation (18). The method is a classical perturbation method that has been used to solve the weak nonlinear differential equation [27]. The solution of equation (18) can be represented by an expansion of \( \eta \), as

\[
\eta = \varepsilon \eta_0(T_0, T_2) + \varepsilon^3 \eta_3(T_0, T_2),
\]

(19)

here \( T_0 = \tau \) and \( T_2 = \varepsilon^2 \tau \). Substituting equation (19) into (17), and equating the coefficients of \( \varepsilon \) and \( \varepsilon^3 \) on both sides, we get the following set of equations [27]:

\[
D_0^2 \eta_0 + k_1^2 \eta_0 = 0,
\]

(20)

\[
D_0^2 \eta_1 + k_1^2 \eta_1 = -2D_0 D_2 \eta_0 - 2\varepsilon D_0 \eta_0 - k_3 \eta_0^3 + f(\pi) \cos (k_1 T_0 + \sigma T_2),
\]

(21)

here \( \omega = k_1 = \varepsilon^2 \sigma \). \( D_0, D_2 \) signify derivatives of \( T_0 \) and \( T_2 \), respectively. According to the ordinary differential equation theory, the solution of equation (20) is

\[
\eta_0 = A(T_2) \exp (ik_1 T_0) + \cc,
\]

(22)

here \( \cc \) denotes the complex conjugate of the preceding term. Substituting \( \eta_0 \) into equation (21), gives

\[
D_0^2 \eta_1 + k_1^2 \eta_1 = -2ik_1(D_2A + cA) + 3k_3A^2 \exp (ik_1 T_0) - k_3 A^3 \exp (3ik_1 T_0) + \frac{1}{2} f \exp [i(k_1 T_0 + \sigma T_2)] + \cc.
\]

(23)

To eliminate secular terms [27] from equation (23), gives

\[
2ik_1(D_2A + cA) + 3k_3A^2 \exp (ik_1 T_0) - \frac{1}{2} f \exp (i\sigma T_2) = 0.
\]

(24)

Let \( A = \alpha \exp (i\beta) / 2 \), where \( \alpha \) and \( \beta \) are real functions of \( T_2 \). Then separating the real and imaginary parts of equation (24), has

\[
D_2 \alpha = -\alpha + \frac{f}{2k_1} \sin (\alpha T_2 - \beta),
\]

(25)

\[
\alpha D_2 \beta = \frac{3k_3}{8k_1} \alpha^3 - \frac{f}{2k_1} \cos (\alpha T_2 - \beta).
\]

(26)

A steady-state motion will occur when \( D_2 \alpha = D_2 \beta = 0 \). And \( \alpha, \beta \) can be obtained through the following nonlinear equations

\[
-\alpha + \frac{f}{2k_1} \sin \gamma = 0, \quad \sigma \alpha - \frac{3k_3}{8k_1} \alpha^3 + \frac{f}{2k_1} \cos \gamma = 0,
\]

(27)
Here $\gamma = \alpha T_2 - \beta$. Equation (27) gives

$$\left[ c^2 + \left( \sigma - \frac{3k_3}{8k_1} \alpha^2 \right)^2 \right] \alpha^2 = \frac{f^2}{4k_1^2}. \quad (28)$$

Equation (28) is an implicit equation for the response amplitude $\alpha$ as a function of the detuning parameter $\sigma$ and the excitation amplitude $f$. There may be two bifurcation points in the frequency-response curve or the excitation amplitude-response curve [27, 28], as shown in figures 3 and 4. The bending of the response curves, which come from the cubic nonlinear terms, leads to multivalued amplitudes and a jump phenomenon at the bifurcation points. The jump phenomenon has physical significance because it leads to a sudden change of vibration amplitudes at the bifurcation points [27]. Substituting $\alpha$ and $\gamma$ into equation (19), has a first-order approximate solution of equation (18)

$$\eta \approx \varepsilon \eta_0 = \varepsilon \alpha \cos (\omega t - \gamma). \quad (29)$$

4. Example and discussion

There is less attention to the damping coefficient of CNTs up to now. $\varepsilon = 0.05$ is used in this paper. A (15, 15) armchair SWCNT is used as an example to discuss the nonlinear stress-strain relationship’s influence on mechanical properties. So we have the diameter $d = 2.034$ nm, the wall thickness $h = 0.34$ nm, and other physical and geometric parameters are $l = 1.115$ nm, $A = 2.171$ nm$^2$, $l = 8$ nm, $m = 4.866 \times 10^{-15}$ kg, and $\omega_0^2 = 5.460 \times 10^4$ s$^{-2}$. Using $E = 1.0$ TPa, $D = -2.0$ TPa [18], has $k_1 = 1$, $k_3 = 11.415$ for $D = -2.0$ TPa, and $k_3 = 31.101$ for $D = 0$. According to equation (17), the amplitude of static bending as a function of the static load can be obtained, as shown in figure 2. And according to equation (28), the vibration amplitude as a function of the excitation frequency or the excitation amplitude can be obtained, as shown in figures 3 and 4. It is found from figure (2) that the nonlinear terms induced by the nonlinear term of strain have a softening response [27, 28]. Under the same loads, this softening response makes that the deformations with the nonlinear stress-strain relationship are larger than that with the linear stress-strain relationship. For the static deformations of the CNTs, when the deformations increase, the nonlinear stress-strain relationship plays an important role, as shown in figure 2. More importantly, the nonlinear terms, which are induced by the quadratic nonlinear term of strain, significantly change the positions of the bifurcation points and dramatically change the oscillation amplitudes, as shown in figures 3 and 4.

It is necessary to note, up to this day, that experiments and atomic calculations of the CNTs’ nonlinear stress-strain relationship are scarce [3, 29]. CNTs were discovered about forty years ago, and early theoretical and
experimental studies focused on the elasticity parameters: Young’s modulus and Poisson’s ratio. The experiments of checking CNTs’ nonlinear stress-strain relationship are more difficult than graphene [30]. From the preliminary results of this paper, it can be found that the nonlinear constitutive relation has a significant effect on the mechanical properties of SWCNTs. SWCNTs have many potential applications, such as scanning probe microscopy and sensors [1, 2], and these applications are related to their mechanical properties. Therefore, we believe that it is necessary to establish the accurate CNTs’ constitutive relationship through experiments and theoretical calculations.

5. Conclusion

In this paper, a new Bernoulli–Euler beam model of SWCNTs has been obtained, for the first time, based on the nonlinear stress–strain relationship obtained from experiments and quantum calculations of graphene. The new model contains a few cubic nonlinear terms induced by the nonlinear stress–strain relationship. The results of static bending and forced vibration show that the nonlinear stress–strain relationship significantly influences the mechanical properties of SWCNTs. It may be necessary to re-examine the SWCNTs’ research results that come from the linear stress–strain relationship.

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ORCID iDs

Kun Huang https://orcid.org/0000-0001-5194-1255

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