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STATIC ANALYSIS OF SINGLE WALLED CARBON NANOTUBES (SWCNT) BASED ON ERINGEN'S NONLOCAL ELASTICITY THEORY

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Abstract

Static analysis of carbon nanotubes (CNT) is presented using the nonlocal Bernoulli-Euler beam theory. Differential quadrature (DQ) method is used for bending analysis of numerical solution of carbon nanotubes. Numerical results are presented and compared with that available in the literature. Deflection and bending moment are presented for different boundary conditions. It is shown that reasonable accurate results are obtained.

Key Words: Carbon nanotubes, static analysis, differential quadrature method, Euler beam, nonlocal elasticity.

1. Introduction

Carbon nanotubes were discovered in 1991 by Sumio Iijima [1]. Carbon Nanotubes (CNT) have a very basic chemical structure. It easy to think of them as small graphene sheets rolled into a cylinder. Carbon nanotubes (CNT) are molecular-scale tubes of graphitic carbon with outstanding properties (Fig. 1). It is accepted that CNT are unique nanostructures with remarkable electronic and mechanical properties. Since the CNT were discovered extensive theoretical and experimental studies on mechanical properties of CNT has been performed [2-10]. Vibration, bending and buckling behavior of CNT has been a subject of interest in the past five years. Molecular dynamics or atomistic model has been used in order to look into the mechanics of nanotubes. Moreover, many authors have employed a continuum or structural mechanics approach for more practical and efficient modeling. For this purpose, rod, beam and shell theories have been used by researchers [11-16]. In the literature, there have been a large number of studies, both theoretical and experimental, of the mechanical properties of carbon nanotubes. Recently, much attention has been devoted to the mechanical behavior of micro/nano structures such as nanobeams, nanorods, nanotubes and microtubules. Beam theories have been always used for modeling of this kind of nanodevices. The main goal of this paper is to present a numerical solution of bending analysis of single walled carbon nanotubes (SWCNT) based on the nonlocal elasticity theory of Bernoulli-Euler beam. To the author knowledge, it is the first time the DQ method has been successfully applied to carbon nanotubes based on linear theory of Bernoulli-Euler beam for the numerical analysis of bending.

2. Differential Quadrature (DQ) Method

Differential quadrature (DQ) method is a relatively new numerical technique in applied mechanics. The method of differential quadrature was proposed to solve linear and nonlinear differential equations and later it was introduced to solid and fluid mechanics by Bert et al. [17,18], Shu and Xue [19], and Civalek [20-23]. The method of DQ can yield accurate solutions with relatively much fewer grid points. It has been also successfully employed for different solid and fluid mechanic problems.

Unlike the DQ that uses the polynomial functions, such as power functions, Lagrange interpolated, and Legendre polynomials as the test functions, harmonic differential quadrature (HDQ) uses harmonic or trigonometric functions as the test functions. Shu and Xue [19] proposed an explicit means of obtaining the weighting coefficients for the HDQ. When the $f(x)$ is approximated by a Fourier series expansion in the form

$$f(x) = c_0 + \sum_{k=1}^{N/2} \left(c_k \cos\frac{k\pi x}{L} + d_k \sin\frac{k\pi x}{L} \right) \tag{1}$$

and the Lagrange interpolated trigonometric polynomials are taken as

$$h_k(x) = \frac{\sin\frac{(x-x_0)\pi}{2}\cdots\sin\frac{(x-x_{k-1})\pi}{2}\sin\frac{(x-x_{k+1})\pi}{2}\cdots\sin\frac{(x-x_N)\pi}{2}}{\sin\frac{(x_k-x_0)\pi}{2}\cdots\sin\frac{(x_k-x_{k-1})\pi}{2}\sin\frac{(x_k-x_{k+1})\pi}{2}\cdots\sin\frac{(x_k-x_N)\pi}{2}} \tag{2}$$

for k = 0,1,2,....,N. According to the HDQ, the weighting coefficients of the first-order derivatives A_{ij} for $i \neq j$ can be obtained by using the following formula:

$$A_{ij} = \frac{(\pi/2)P(x_i)}{P(x_j)\sin[(x_i - x_j)/2]\pi}; \quad i,j = 1,2,3,...,N, \tag{3}$$

Where

$$P(x_i) = \prod_{j=1, j\neq i}^{N} \sin\left(\frac{x_i - x_j}{2}\pi\right); \quad \text{for } j = 1,2,3,...,N. \tag{4}$$

The weighting coefficients of the second-order derivatives B_{ij} for $i \neq j$ can be obtained using following formula:

$$B_{ij} = A_{ij}\left[2A_{ii}^{(1)} - \pi ctg\left(\frac{x_i - x_j}{2}\right)\pi\right]; \quad i,j = 1,2,3,...,N, \tag{5}$$

The weighting coefficients of the first-order and second-order derivatives $A_{ij}^{(p)}$ for $i = j$ are given as

$$A_{ii}^{(p)} = -\sum_{j=1, j\neq i}^{N} A_{ij}^{(p)}\ ; p = 1 \text{ or } 2\ ; \text{and for } i = 1,2,..., N. \tag{6}$$

A natural, an often convenient, choice for sampling points is that of equally spaced point. It was also reported that the Chebyshev-Gauss-Lobatto or non-equally sampling grid (NE-SG) points for spatial discretization as;

$$x_i = \frac{1}{2}[1 - \cos(\frac{i-1}{N-1})\pi] \tag{7}$$

performed consistently better than the equally spaced.

Fig. 1. Typical single-walled carbon nanotubes

For more details of the mathematical background and application of the DQ method in solving problems in engineering, the readers may refer to some recently published reference [18-23].

3. Beam Modeling Of SWCNTs

A typical single walled carbon nanotubes (SWCNTs) based on beam theory is depicted in Fig. 2. In this figure, the letter *d* is the diameter of beam, L length of the beam.

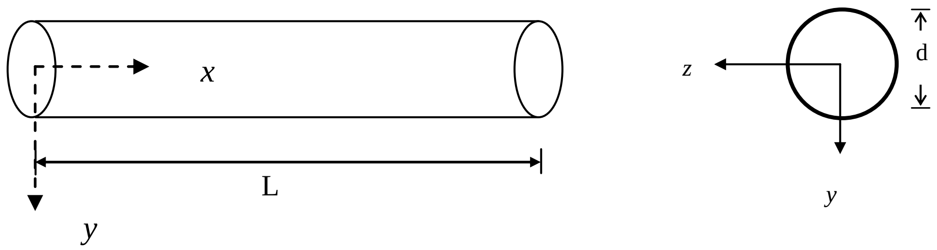

Fig. 2. Single-walled CNT

For transversely vibration of carbon nanotubes, the equilibrium conditions of Euler-Bernoulli beam can be written as

$$\frac{\partial V(x,t)}{\partial x} = \rho A \frac{\partial^2 w(x,t)}{\partial t^2} \tag{8}$$

$$V(x,t) = \frac{\partial M(x,t)}{\partial x} \tag{9}$$

where $V(x,t)$ and $M(x,t)$ are resultant shear force and bending moment of the beam, ρ the mass density, A the area of the cross-section of the beam, $w(x,t)$ is the transverse displacement of the microtubules and t the time variable. We obtain the following relation from Eqs (8) and (9)

$$\frac{\partial^2 M(x,t)}{\partial x^2} = \rho A \frac{\partial^2 w(x,t)}{\partial t^2} \tag{10}$$

According to the linear theory of Euler-Bernoulli beam, the strain-displacements and the moment are given by

$$\varepsilon = -y \frac{\partial^2 w(x,t)}{\partial x^2} \tag{11}$$

$$M(x,t) = \int_A y\sigma dA \tag{12}$$

For bending analysis by writing the equilibrium equation for the vertical force for infinitesimal Euler-Bernoulli beam under uniformly distributed load, we obtain

$$\frac{dV(x,t)}{dx} + q(x) = 0 \tag{13}$$

The moment equilibrium are also written as

$$V(x,t)dx - M(x,t) + M(x,t) + dM(x,t) - q(x) \times dx \times dx / 2 = 0 \tag{14}$$

Then we obtain

$$V(x,t) - \frac{dM(x,t)}{dx} = 0 \tag{15}$$

Substituting this into (13), we obtain

$$q(x) + \frac{d^2 M(x,t)}{dx^2} = 0 \tag{16}$$

The statements for bending moment and shear force are given as

$$M(x,t) = -EI\,\frac{\partial^2 w(x,t)}{\partial x^2} = 0 \tag{17}$$

$$V(x,t) = -EI\,\frac{\partial^3 w(x,t)}{\partial x^3} = 0 \tag{18}$$

According to the nonlocal elasticity theory of Eringen's [28], the stress at any reference point in the body depends not only on the strains at this point but also on strains at all points of the body. This definition of the Eringen's nonlocal elasticity is based on the atomic theory of lattice dynamics and some experimental observations on phonon dispersion. In this theory, the long range force about atoms is considered and thus internal scale effect is introduced in the constitutive equation. In this theory, the fundamental equations involve spatial integrals which represent weighted averages of the contributions of related strain tensor at the related point in the body. Thus theory introduces the small length scale effect through a spatial integral constitutive relation. For homogenous and isotropic elastic solids, the linear theory of nonlocal elasticity is described by the following equations:

$$\sigma_{kl,l} + \rho(f_l - \frac{\partial^2 u_l}{\partial t^2}) = 0, \tag{19}$$

$$\sigma_{kl}(x) = \int_V \alpha(|x - x'|, \chi)\tau_{kl}(x')dV(x'), \tag{20}$$

$$\tau_{kl}(x') = \lambda\varepsilon_{mm}(x')\delta_{kl} + 2\mu\varepsilon_{kl}(x'), \tag{21}$$

$$\varepsilon_{kl}(x') = \frac{1}{2}\left(\frac{\partial u_k(x')}{\partial x'_l} + \frac{\partial u_l(x')}{\partial x'_k}\right), \tag{22}$$

where σ_{kl} is the nonlocal stress tensor, ρ is the mass density of the body, f_l is the body (or applied) force density, u_l is the displacement vector at a reference point x in the body, $\tau_{kl}(x')$ is the classical (Cauchy) or local stress tensor at any point x' in the body, $\varepsilon_{kl}(x')$ is the linear strain tensor at point x' in the body, t is denoted the time, V is the volume occupied by the elastic body, $\alpha|x - x'|$ is the distance in Euclidean form, λ and μ are the Lame constants. The non-local kernel $\alpha|x - x'|$ defines as the impact of the strain at the point x' on the stress at the point x in the elastic body. The value of χ depends on the ratio ($e_0 a / l$) which is material constant. The value a depends on the internal (granular distance, lattice parameter, distance between C-C bonds as molecular diameters) and external characteristics lengths (crack length or wave length) and e_0 is a constant appropriate to each material for adjusting the model to match reliable results by experiments or some other theories. For an elastic beam in the one dimensional case, the nonlocal constitutive relations can be written as below

$$\sigma_{xx} - (e_0 a)^2 \frac{\partial^2 \sigma_{xx}}{\partial x^2} = E\varepsilon_{xx} \tag{23}$$

For a uniformly distributed load the related equations can be written as

$$V(x) = -EI \frac{d^3 w(x)}{dx^3} = -qx - c_1 \tag{24}$$

$$M(x) = -EI \frac{d^2 w(x)}{dx^2} - (e_0 a)^2 q = -qx^2/2 - c_1 x - c_2 \tag{25}$$

where c_i (i=1,…,4) are constant of integration which must be determined using the related boundary conditions of the microtubules. If we consider the Euler-Bernoulli beam subjected to a distributed load and series of concentrated loads P_i at $x = x_i$ (*i*=1,2,…,*n*), the general nonlocal equation for this case is given below [24]

$$EI \frac{\partial^4 w(x)}{\partial x^4} + q(x)(e_0 a)^2 \frac{\partial^2 q(x)}{\partial x^2} - q(x)$$

$$+ q(x)(e_0 a)^2 \frac{\partial^2 q(x)}{\partial x^2} + \sum_{i=1}^{n} P_i \left[\delta(x - x_i) - (e_0 a)^2 \delta''(x - x_i)\right] \tag{26}$$

where δ is the Dirac delta function and defined as

$$\delta(x - x_i) = \begin{cases} \infty, & x = x_0 \\ 0, & \text{otherwise} \end{cases} \tag{27}$$

Three-types of boundary conditions are considered. These are:

For simply supported(S) end : $W = 0$ and $M = 0$ (28a)

For clamped (C) end: $W = 0$ and $dW/dx = 0$ (28b)

For free (F) end: $V = 0$ and $M = 0$ (28c)

4. Results

In this section, a number of numerical examples are given to illustrate the application of the present method. The material and geometric constant of CNT are taken as: L=10 nm, E=2*10^9 N/m^2, I=64,33*10^{-36} m^4. A uniformly distributed load has been considered for three different boundary conditions. For clamped CNT, deflection profile is shown in Figure 3. As expected maximum deflection is obtained on the center of the beam.

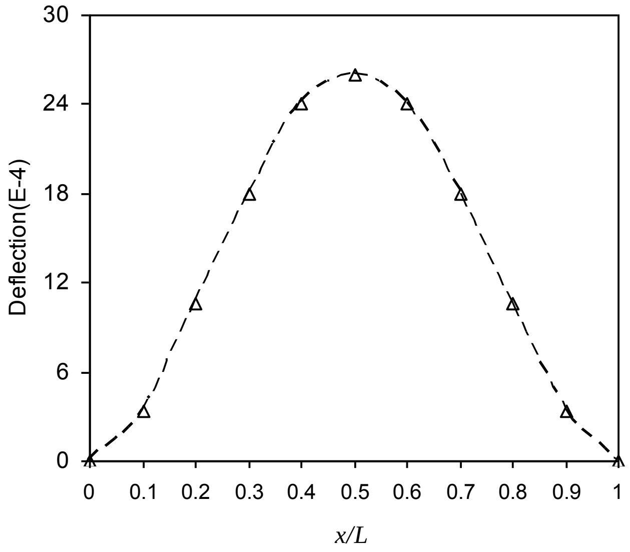

Fig. 3. Non-dimensional deflection (EI/ql^4) of C-C SWCNT

In Figure 4, non-dimensional deflection for C-C carbon nanotubes is depicted for different value of load. It may be concluded that decreasing the load, *q* will always result in decreased deflection. In figure 5, three-different boundary conditions are taken into consideration for bending of carbon nanotubes. It is clearly shown that the deflection response of C-F nanotubes is higher than the response of C-C and S-S carbon nanotubes.

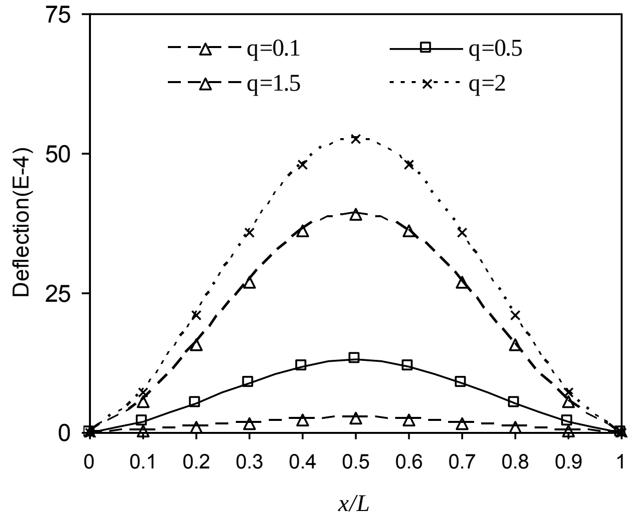

Fig. 4. Non-dimensional deflection (EI/l^4) of C-C SWCNT for different loading

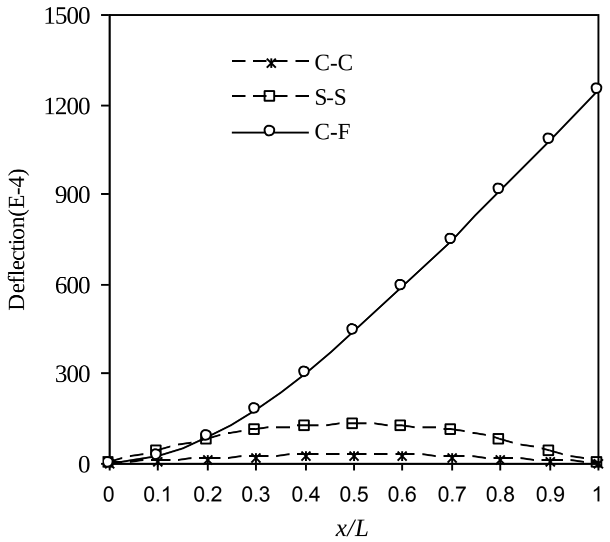

Fig. 5. Non-dimensional deflection (EI/l^4) of SWCNT for different boundary conditions

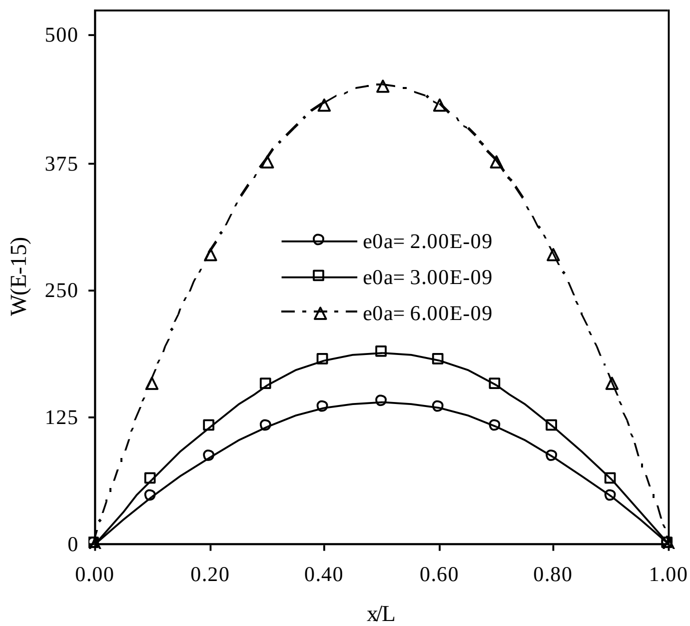

Fig. 6. Static deformation of S-S carbon nanotubes for different nonlocal parameters

5. Conclusions

By using the Euler-Bernoulli beam theory, DQ based numerical approach for deflection and bending analysis of single walled carbon nanotubes is investigated. Some numerical examples were provided. Although not provided here, the method is also useful in providing nonlinear behaviour of single-walled carbon nanotubes [26,27]. The present study is being further developed to overcome the convergence problems encountered in the nonlinear static and buckling analysis of carbon nanotubes.

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