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Nonlocal Elasticity Theory for Free Vibration of Single-walled Carbon Nanotubes

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Abstract. This paper concerns with free vibration analysis of single-walled carbon nanotubes including the effect of small length scale based on the nonlocal elasticity theory. The governing equation of nanotube is derived from Euler beam theory including a nonlocal parameter in the function of masses. Classical solutions are obtained and then compared with the numerical solutions provided by finite element models. Effect of tube chirality and various geometrically boundary conditions are considered. The finite element models of nanotubes are assumed as the virtually analogous frame structures. In the numerical technique, the atomic masses existing on the both ends of beams are assigned by physical and chemical properties of carbon element. The results show that the natural frequencies significantly increase when the nonlocal parameters decrease. The numerical results are in good agreement with the classical solutions for the nanotubes with low aspect ratios and are acceptable for high aspect ratios. Furthermore, the first-ten mode shapes are demonstrated for various aspect ratios and boundary conditions, and the repeated natural frequencies are also highlighted in this study.

Introduction

Since carbon nanotubes (CNTs) had been discovered by Iijima [1] in 1991, extensive researches had been done to obtain their extraordinary properties such as a high aspect ratio and flexibility [2], a very large tensile strength and Young modulus [3], superconductivity and well-bonding strength between carbon atoms. Free vibration analysis of CNTs using beam element [4] has been studied to obtain the properties and behaviors of materials and those results are validated by the other methods. Although the results from the classical beam theory gave the exact closed-form solutions, however in many cases it is necessary to have the results from the conventional numerical methods as alternative approaches to verify these results.

In this work, the effect of small length scale based on the nonlocal elasticity is included in the equation of motion of nanotube based on Euler beam theory. Finite element models of single-walled carbon nanotubes (SWCNTs) are also developed as the frame-like structures in order to validate the results from the classical method.

Equation of motion of nonlocal carbon nanotube

According to Eringen [5], the nonlocal theory is based on the crucial concept that stress at a point is a function of strains at all points in the continuum. It is quite different from the conventional theory that the stress at the point depends only on the strain at the point. Based on the conditions of a homogeneous isotropic beam in one dimensional analysis to simplify the problem, the nonlocal constitutive relations can be expressed as

$$\sigma_{xx} - \mu \frac{\partial^2 \sigma_{xx}}{\partial x^2} = E\varepsilon_{xx} \quad (1)$$

where σ_{xx}, ε_{xx} and E are a normal stress, a normal strain and Young's modulus, respectively. The scaling factor $\mu = e_0^2 \ell_i^2$ is the function of material constant, it consists of e_0 and ℓ_i that are the material constant and internal characteristic lengths (such as the lattice spacing). In general, it is called the nonlocal parameter which is a factor to consider the effect of small length scale. According to Reddy and Pang [6], this parameter has been used in the classical method to investigate the bending, buckling and free vibration problems of beams. Based on the Euler's beam theory, the equation of motion for free vibration of nanotube including the nonlocal elasticity can be written as

$$m(x)\mu \frac{\partial^2 u}{\partial t^2} + \frac{\partial^2}{\partial x^2}\left[EI(x)\frac{\partial^2 u}{\partial x^2} \right] = 0 \quad (2)$$

where m, I and u are the mass per unit length, the moment of inertia and the transverse displacement, respectively. By using method of separated variables, Eq. 2 yields two ordinary differential equations; one is time dependent equation, the other one is spatial coordinate dependent equation. In case of a uniform cross-section element, the infinite set of frequency parameter β and the associated mode shape $\phi(x)$ that satisfies the eigenvalue problem [7] defined by

$$\phi^{IV}(x) - \beta^2 \phi(x) = 0 \quad (3)$$

when

$$\beta^4 = \frac{\omega^2 \mu m}{EI}. \quad (4)$$

Thus, the general solution of fourth-order ordinary differential equation for Eq. 3 is

$$\phi(x) = C_1 \sin \beta x + C_2 \beta \cos \beta x + C_3 \sinh \beta x + C_4 \cosh \beta x \quad (5)$$

where $C_1, C_2, C_3,$ and C_4 are the unknown constants to be determined from the boundary conditions of the physical problem. For Eq. 4, ω is the natural frequency of free vibration. The various end conditions namely Clamped-Free (C-F), Simply-Simply supported (S-S), Clamped-Simply supported (C-S) and Clamped-Clamped (C-C) are considered in this study. Finite element (FE) models have been assumed as an analogous frame for the structural system that atoms and covalent bond are represented as nodes and beam elements [8,9]. The chemical properties of carbon, the atomic mass is $1.9943 \times 10^{-23}\,g$ that is assigned on the ends of beam element in the FE models and atomic density is 1.36169×10^{-16} *nN/Å³* [5]. For the mechanical properties, Young's modulus, shear modulus, and Poisson's ratio are taking as 10.0 *nN/Å²*, 4.0 *nN/Å²*, and 0.3, respectively. In addition, the nonlocal parameters μ varying from 0.01-0.04 and 0.1-0.4 have been used to exhibit the trend of size effect when comparing those results obtained from the classical method and the FE models.

Results and discussion

Fig. 1 shows that the fundamental frequencies (GHz) versus aspect ratios (L/d) of the SWCNTs with various boundary conditions. It is found that the natural frequencies are significantly depended

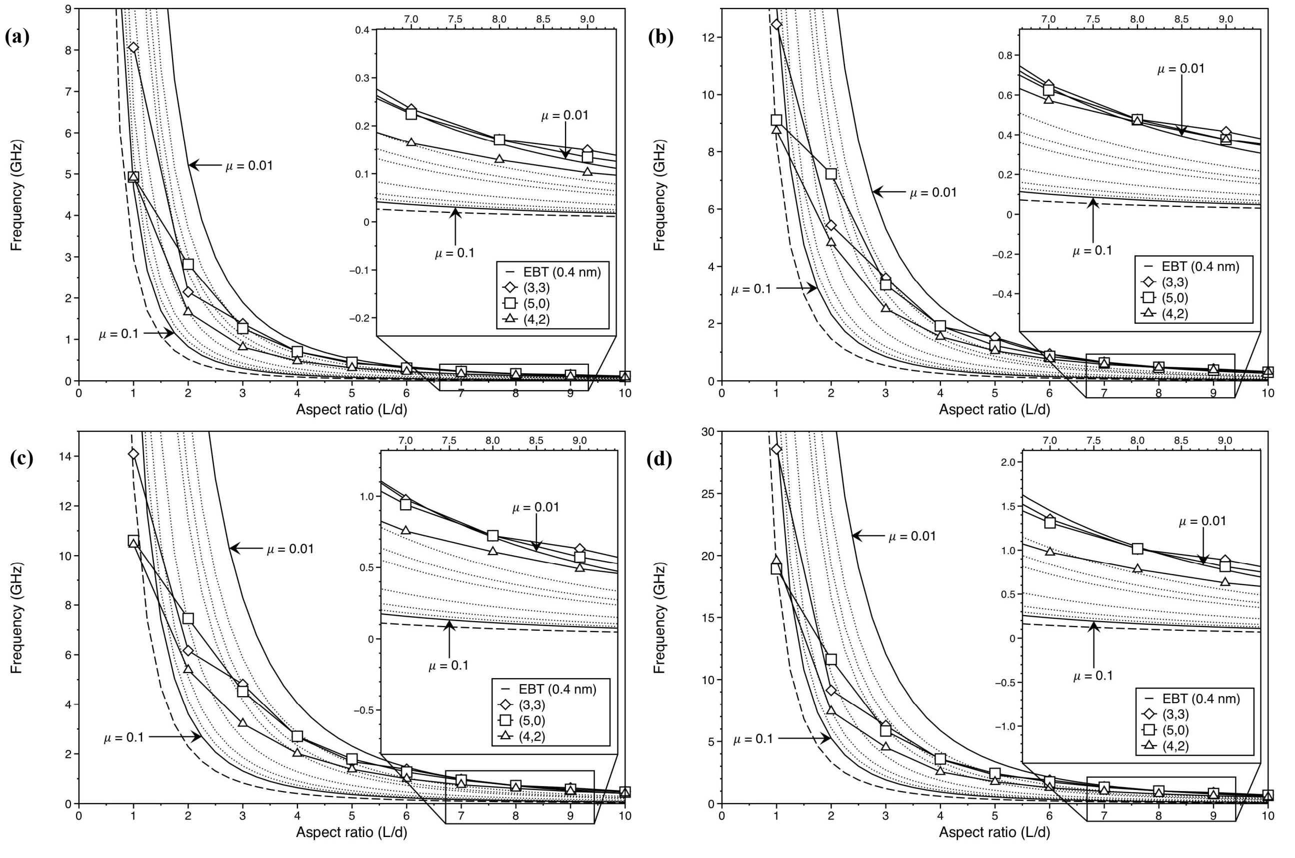

Figure 1. Fundamental frequencies of small diameter (0.4 nm) under the various boundary conditions: (a) C-F, (b) S-S, (c) C-S and (d) C-C

on the boundary conditions and aspect ratios of tube. The results of $\mu = 0.01$ show that they are well acceptable as compared to those results from the FE models with the high aspect ratio (L/d > 6) as shown in the magnified area. For the results of $\mu = 0.1$, both methods are well correlated for the low aspect ratio (L/d < 2). For intermediate aspect ratios (2 < L/d <6), the results from the FE models lie in between the nonlocal parameters (μ > 0.01 and μ > 0.1). For example, the results with aspect ratio L/d = 5 are close to the values at $\mu = 0.02$ as shown in Fig. 1(d).

In cases of higher modes, the numerical results are exhibited on Table 1 for $\mu = 0.1$. The repeated frequencies occur in many nearby mode shapes. For example, the repeated frequency of nanotube (9,9) $\omega_{C-C} = 2.6637$ GHz is found at the 3rd and 4th modes as shown in the last column on Table 1. In addition, the first-ten mode shapes with various boundary conditions are also presented in Fig. 2.

Table 1. The natural frequencies for the first-ten mode with various conditions for μ =0.1

Tube (*n,m*)	(3,3)	(9,9)	(5,0)	(26,0)	(12,6)	(20,10)	(3,3)	(9,9)
dia. (*nm*)	0.4	1.2	0.4	2.0	1.2	2.0	0.4	1.2
L (*nm*)	3.6	3.6	4.0	4.0	6.0	6.0	2.4	2.4
L/d	9	3	10	2	5	3	6	2
B.C.	C-F	C-F	S-S	S-S	C-S	C-S	C-C	C-C
Mode no.								
1	0.1493	0.3672	0.3031	0.9938	0.4615	0.5740	1.8897	2.5027
2	0.1493	0.3673	0.5943	0.9957	0.5053	0.6008	1.8901	2.5033
3	0.8720	1.2219	1.1501	1.0222	0.8071	0.7204	3.8234	2.6637
4	0.8724	1.4982	1.5723	1.1345	1.2071	0.7245	4.4458	2.6637
5	1.2136	1.4983	2.1251	1.8630	1.2010	0.7785	4.4463	3.8534
6	1.5022	1.4990	2.4466	1.9476	1.3188	1.0614	4.6379	4.5947
7	2.2338	1.7975	2.4469	1.9741	1.7538	1.0702	7.5953	4.5950
8	2.2349	1.7976	2.9093	1.9843	1.7555	1.2726	7.5984	4.5991
9	3.6464	2.1875	3.9476	2.2220	1.9551	1.3196	7.6890	4.6675
10	3.9586	2.1876	4.2546	2.2974	1.9608	1.3436	9.2057	4.6678

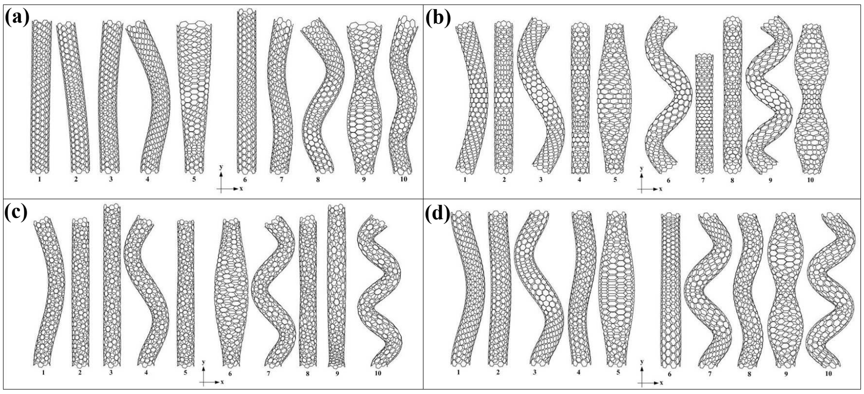

Figure 2. The first-ten mode shapes depending on the boundary conditions: (a) C-F, (b) S-S, (c) C-S and (d) C-C

Summary

The equation of motion for the free vibration analysis of CNTs including the effect of nonlocal elasticity has been considered in this study. The numerical results based on FE models are in good agreement with those obtained from the classical method. It can be concluded that the natural frequencies generally depend on atomic arrangements, tube lengths, tube diameters and boundary conditions. Furthermore, the natural frequencies increase with the decrease in the nonlocal parameters μ and the repeated frequencies with different mode shapes are found in many places for various cases of the boundary conditions.

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