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Computation of Carbon Nanotubes Eigenfrequencies Based on Nonlocal Theory and Using Finite Element Method

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Abstract. In this paper the eigenfrequencies of carbon nanotubes are investigated. Especially, effect of chirality of the carbon nanotubes is studied. The effect of the change of chiral angle is investigated for the carbon nanotubes with the same diameter, length and two different types of boundary conditions. The nonlocal continuum theory results to application of nonlocal parameter which has influence to eigenfrequencies of carbon nanotubes. All computations in the paper are made by finite element method, where standard mass matrix of finite element is corrected and updated by nonlocal parameter.

Introduction

Carbon nanotubes (CNTs) are closed graphene sheets of cylindrical shape with interesting mechanical properties. Especially, high tensile strength and stiffness in relation to very small weight attracts attention of engineers and researches. Three basic methods of nanotubes investigation are used to accomplish simulation of SWCNTs: molecular dynamic computations, atomistic-based modelling and the continuum approach. The last one is used here for description of bending vibration and accordingly it can serve as a mean tool for indirect specification of carbon nanotube properties. The continuum beam relations used in the paper are based on the theory of nonlocal elasticity published by Eringen [1]. The equations are solved by the finite element method.

In this paper the finite element modal analysis of the CNTs is performed. The effect of chirality, dimensions and nonlocal parameter on the eigenfrequencies of CNTs is investigated. The matrix formulations of the stiffness matrix and mass matrix of finite element is used for the modelling and computations of CNTs. The effect of nonlocal parameter is represented by the coefficient used in the mass matrix.

Finite element modelling of carbon nanotubes

In contrast to the classical elasticity theory Eringen takes into account the scale effect and its influence to stress at the reference point of a body. Accordingly, the stress at a point is a function of strain field at every point of body. Review of nonlocal elastic models of CNTs is given in [1]. The interesting results of CNT research can be found in literature [1]-[6]. The nonlocal finite element formulation is presented for computation of eigenfrequencies of CNTs. The mass and stiffness matrices of finite element are derived from equation

$$m_b(x)\mu\frac{\partial^2 u}{\partial t^2}+\frac{\partial^2}{\partial x^2}\left[EJ(x)\frac{\partial^2 u}{\partial x^2}\right]=0. \tag{1}$$

Here, u is the transverse displacement of the beam, m_b is the mass of beam related to the unit length, μ is nonlocal parameter, E is Young modulus, J is the second moment of cross-section area, x is a coordinate of point in beam nanotube, t is time.

As there is a problem in definition of thickness of the nanotubes, the values necessary for computations were determined according to [4] as

$$m = \rho A = 2.4 \times 10^{-24} D \quad [\mathrm{kg/nm}], \tag{2}$$

$$EI = 428.48 D^2 - 397.08 D + 109.24 \quad \left\lfloor \mathrm{kg\,nm^3/s^2} \right\rfloor, \tag{3}$$

where D is a diameter of nanotube. The nanotube diameter can be computed from equation

$$D = 2R = a_0 \sqrt{3(m^2 + n^2 + mn)} / \pi, \tag{4}$$

where $a_0 = 1.42$ $\mathring{A}$ is a carbon–carbon bond length and the integers m and n are called as chiral indices. There are known three configuration types of chiral indices called as armchair (m, m), chiral (m, n) and zigzag (m, 0). Here, for armchair nanotube we have $m = n$.

For the modelling of CNTs, we have used plane beam element with four degrees of freedom, length l_e and mass m_b. The basic FEM matrices are formulated by standard matrix of shape functions $\mathbf{N}(x)$. Then, the element stiffness and mass matrices can be defined respectively by equations

$$\mathbf{K}_e = EJ \int_0^{l_e} \frac{d^2\mathbf{N}(x)}{dx^2} \frac{d^2\mathbf{N}^T(x)}{dx^2} dx = \frac{EJ}{l_e^3} \begin{bmatrix} 12 & 6l_e & -12 & 6l_e \\ 6l_e & 4l_e^2 & -6l_e & 2l_e^2 \\ -12 & -6l_e & -12 & -6l_e \\ 6l_e & 2l_e^2 & -6l_e & 4l_e^2 \end{bmatrix}, \tag{5}$$

$$\mathbf{M}_e = m_b \mu \int_0^{l_e} \frac{d^2\mathbf{N}(x)}{dx^2} \frac{d^2\mathbf{N}^T(x)}{dx^2} dx = \frac{m_b \mu l_e}{420} \begin{bmatrix} 156 & 22l_e & 54 & -13l_e \\ 22l_e & 4l_e^2 & 13l_e & -3l_e^2 \\ 54 & 13l_e & 156 & -22l_e \\ -13l_e & -3l_e^2 & -22l_e & 4l_e^2 \end{bmatrix}. \tag{6}$$

At first, the effect of chirality to eigenfrequencies of CNTs is investigated. The computations of the first two eigenfreqeuncies are accomplished for different types of CNTs but with approximately the same diameters. The length of tubes is 10 nm and the following types of boundary conditions are used: fixed–free (F–Fr) and simply–simply supported (S–S). From computations (Table 1) we see that the chirality has effect to the results mainly due to small change of tube diameter. Under otherwise identical conditions, the effect of chirality of SWCNTs is negligible. For this reason, only armchair CNTs with chirality (m, m) are investigated in this paper.

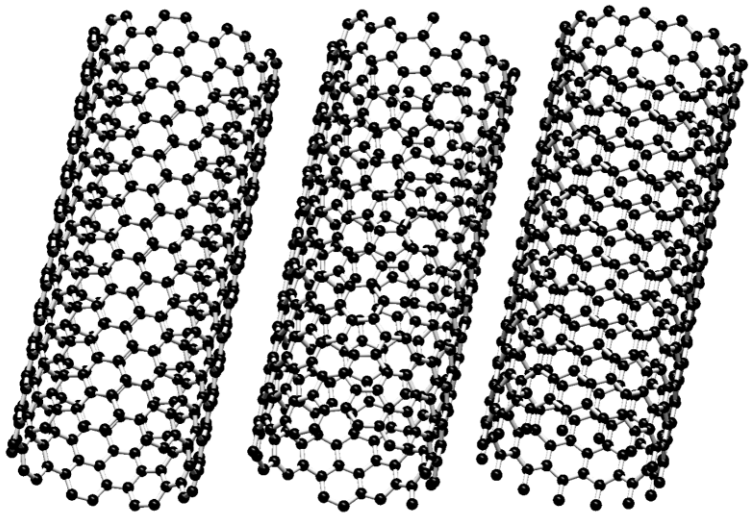

Fig.1 Types of carbon nanotubes

Tab.1 Eigenfrequencies of CNTs with different chiral angles and boundary condition

SWCNT (n, m)	Chiral angle (°)	Diameter (nm)	Frequency (THz)			
			F-Fr (1^{st})	F-Fr (2^{nd})	S-S (1^{st})	S-S (2^{nd})
(9, 0)	0.00	0.7047	0.02795	0.17515	0.07845	0.31381
(8, 2)	10.89	0.7177	0.02858	0.17912	0.08023	0.32092
(7, 3)	17.00	0.6960	0.02753	0.17249	0.07726	0.30905
(6, 4)	23.41	0.6826	0.02689	0.16852	0.07548	0.30192
(5, 5)	30.00	0.6781	0.02668	0.16719	0.07489	0.29955

The four CNTs with the same chirality (*m*, *m*) but different diameters are modelled (Table 2). These CNTs are modelled with lengths varying from 10 nm to 100 nm and the finite element modal analysis is performed on these CNTs. Due to big amount of data, the results are given only for the first and the fifth eigenfrequency of CNTs with fixed-free boundary conditions and they are presented in Figs. 2-3. From the figures can be seen that the bigger diameter of the CNT leads to the higher eigenfrequency and the longer CNT leads to the smaller eigenfrequency.

Tab.2 Modelled carbon nanotubes

SWCNT (m, m)	Chiral angle (°)	Diameter (nm)
(5, 5)	30.00	0.6785
(10, 10)	30.00	1.357
(20, 20)	30.00	2.714
(40, 40)	30.00	5.428

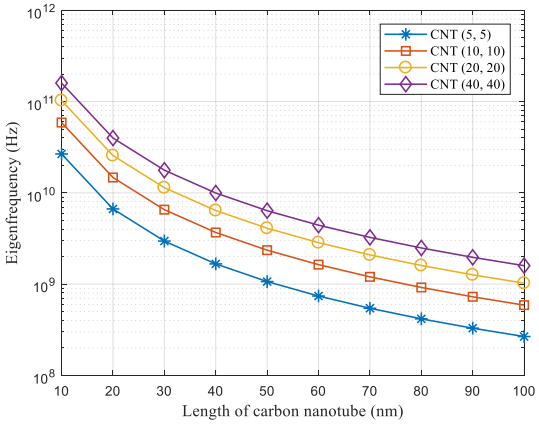

Fig. 2 The first eigenfrequencies of carbon nanotubes

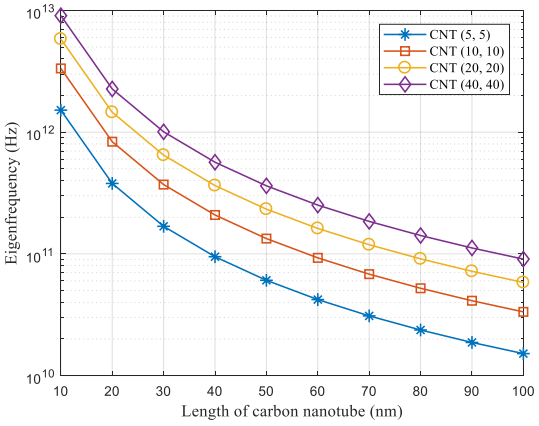

Fig. 3 The fifth eigenfrequencies of carbon nanotubes

Next, the effect of nonlocal parameter to the eigenfrequencies of CNTs is studied. The computations are accomplished for nonlocal parameters 0.01, 0.1, 0.2, 0.4, 1.2. The CNTs with the chirality (10, 10), the diameter D = 1.357 nm and the lengths from 10 to 100 nm are modelled. In the Figs. 4 – 7 are shown the first four eigenfrequencies with and without nonlocal parameter and for the fixed-free boundary conditions. From the figures can be seen that the nonlocal parameter significantly affects the eigenfrequencies of the CNTs. The nonlocal parameter smaller than one leads to higher eigenfrequencies as the eigenfrequencies computed without nonlocal parameter and the nonlocal parameter higher than one leads to smaller eigenfrequencies as the ones computed without nonlocal parameters. The nonlocal parameters smaller than one have more pronounced effect on the value of the eigenfrequencies.

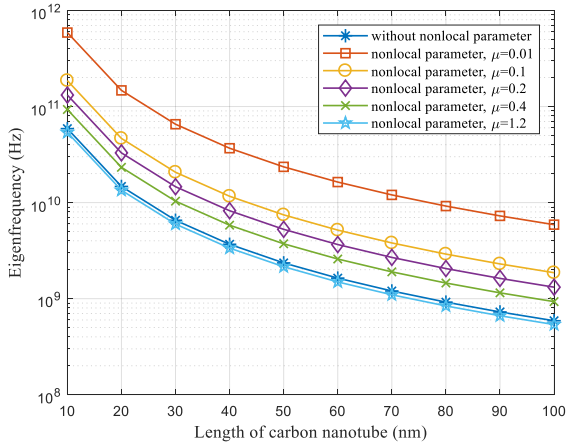

Fig. 4 The first eigenfrequencies of carbon nanotubes with and without nonlocal parameter

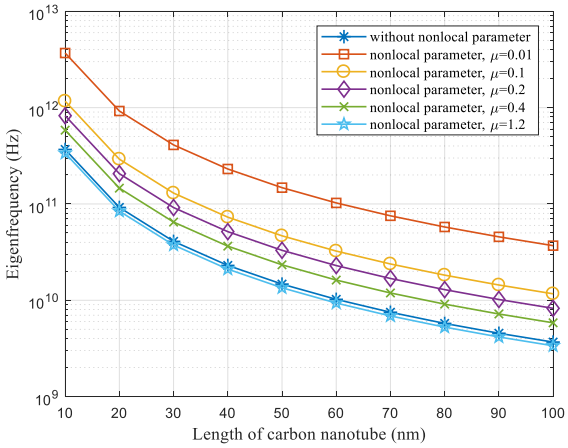

Fig. 5 The second eigenfrequencies of carbon nanotubes with and without nonlocal parameter

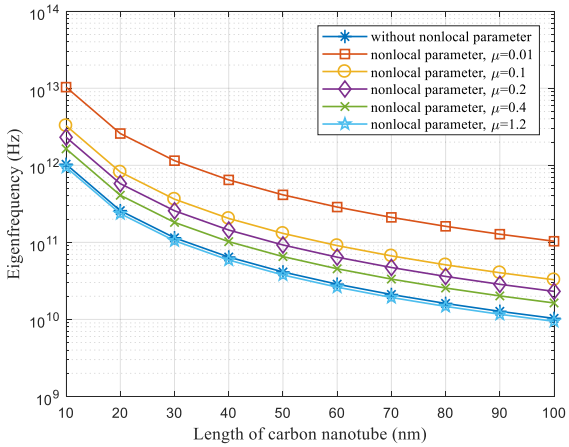

Fig. 6 The third eigenfrequencies of carbon nanotubes with and without nonlocal parameter

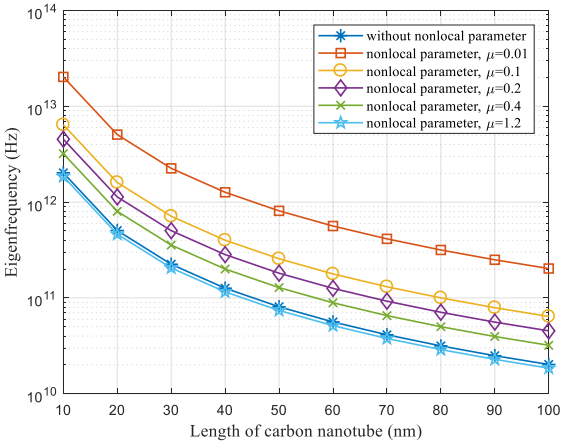

Fig. 7 The fourth eigenfrequencies of carbon nanotubes with and without nonlocal parameter

Conclusions

In the paper are described numerical computations of eigenfrequencies of carbon nanotubes accomplished for different nonlocal parameters, chirality, lengths and boundary conditions. At first, the influence of chiral angle on the values of eigenfrequencies was studied. From computations result that the eigenfrequencies of CNTs with the same diameters and lengths were not affected by the chiral angle. Next, the effect of nonlocal parameter was studied. From the results can be stated that the value of nonlocal parameter affected the eigenfrequencies. In general, the smaller value of the nonlocal parameter, the higher eigenfrequency of nanotube. Computation of eigenfrequencies of carbon nanotubes can serve as a very important tool for determination of basic material properties of homogenized nanotubes, because it is much easier to measure frequencies of nanotubes as e.g. their Young modulus, or other properties. Accordingly, the eigenfrequencies serve for indirect determination of material and geometric properties of nanotubes.

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