Nonlocal beam model and FEM of free vibration for pristine and defective CNTs

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Abstract: The natural frequencies of defective single-walled carbon nanotubes are studied and compared with the values for pristine structures. In order to capture the size-dependent effects in carbon nanotubes, nonlocal stress gradient theory within a Euler-Bernoulli beam model is involved. The analytical computations are compared with finite element analysis of a structural model of carbon nanotubes. The numerical analysis of free vibrations is applied to predict the value of the nonlocal parameter. The eigenfrequencies obtained from finite element analysis are much lower compared with analytical computations of local (classical) beam model. For defective structures having small vacancy, a slight decrease in the eigenfrequencies is observed. All studied boundary conditions indicated the higher the nonlocal parameter is, the lower the natural frequencies are.

1. Introduction

Clamped-clamped and cantilevered carbon nanotube (CNT) resonators have received much attention and make them appropriate as extremely sensitive mass sensors and signal processing units [1,2]. Dynamic characteristic at the atomic level has key influence on nanostructure behavior because of their ultrahigh or very high natural frequencies even in THz [1,3]. For some nano-electromechanical systems, the oscillation frequency is a principal property. Additionally, the natural frequencies or shape modes can be used as the indirect method of the effective Young's modulus evaluation [3].

The application of classical (local) beam models are insufficient in the free vibration analysis of nanostructures. The classical mechanics cannot capture the small scale effect because of scale-free relations. In the studies on the dynamic behavior of CNTs instead of local mechanical models, the nonlocal descriptions are introduced considering the small scale [4,5,6,7,8].

The experimental studies on mechanical properties of CNTs showed that theoretical predictions generate higher values then-experimental ones [9]. It can be explained by defect existence [3]. Considering quasi one-dimensional CNT structure, even a small number of vacancies can influence on the mechanical characteristic [10].

In the present work, the local (classical) and nonlocal vibrational behavior of CNTs based on the Euler-Bernoulli beam theory is presented. Additionally, numerical structural FEM model of pristine and defective CNT is applied in dynamic analysis. Here, we propose the determination of the nonlocal parameter based on the structural finite element model of the nanotube instead of commonly used molecular dynamics (MD) simulations.
2. Fundamental relations for local and nonlocal Euler-Bernoulli beam theory

The local (classical) Euler-Bernoulli beam equation of motion of free vibration in carbon nanotubes is given by:

\[ \rho A \frac{\partial^2 w}{\partial t^2} + EI \frac{\partial^4 w}{\partial x^4} = 0 \]  \hspace{1cm} (1)

where \( t \) – time, \( x \) – axial coordinate; \( w \) – deflection, \( A \) – cross-sectional area, \( \rho \) – mass density, \( E \) – Young’s modulus and \( I \) – moment of inertia. The use of the method of separation of variables in Eq (1) gives two ordinary differential equations, one is a time-dependent equation, the other one is a spatial coordinate dependent equation. The infinite set of frequency parameter \( k \) and the associate mode shape \( X(x) \) that satisfies eigenvalue problem is defined by:

\[ X''''(x) - k^2 X(x) = 0 \]  \hspace{1cm} (2)

when the coupling relation between vibrational frequency \( \omega \) and frequency parameter \( k \) is as follows:

\[ \omega^2 = k^4 \frac{EI}{\rho A} \]  \hspace{1cm} (3)

The general solution of the fourth-order ordinary differential equation (2) is:

\[ X(x) = A \sin kx + B \cos kx + C \sinh kx + D \cosh kx \]  \hspace{1cm} (4)

where \( A, B, C, D \) are unknown constants computed based on boundary conditions. The boundary conditions for nanobeam having length \( L \) are written as: (i) for simply supported (S-S): \( X(0) = X(L) = 0, X''(0) = X''(L) = 0 \), (ii) for clamped-clamped (C-C): \( X(0) = X(L) = 0, X'(0) = X'(L) = 0 \), (iii) for clamped-free (C-F): \( X(0) = X'(0) = 0, X''(L) = X'''(L) = 0 \).

Eringen [11] first introduced the nonlocal elastic continuum mechanics defining that the stress state at a given point depends not only on the local stress at that point but also is as a function of the stress state at all points in the body. The nonlocal Euler-Bernoulli beam equation of motion of free vibration in CNTs is given by:

\[ \rho A \frac{\partial^2 w}{\partial t^2} - (e_0 a^2) \frac{\partial^2 w}{\partial x^2} + EI \frac{\partial^4 w}{\partial x^4} = 0 \]  \hspace{1cm} (5)

where \( e_0 \) – nonlocal material parameter, \( a \) – characteristic internal length. For \( e_0 a = 0 \) we have the local Euler-Bernoulli beam equation. The most important issue in the nonlocal analysis is to determine the magnitude of the nonlocal parameter. The value of the parameter \( e_0 a \) has a significant influence on the final results, and the nonlocal effect is particularly visible for short nanotubes [12,13]. The broad literature review of the nonlocal parameter is presented by Chwał in [14] and will be not discussed here again.

3. Structural finite element model of carbon nanotubes

To investigate the dynamic behavior of carbon nanotubes an exact structural model of single-walled nanotube based on the molecular structural mechanics, continuum mechanics and FEM was built. The numerical model involves the assumption proposed in [15] and [16] in which the nanotube structure, when loaded, behaves like space truss structure. For details see also [14]. Atoms in nanotube create a network made of hexagons (Fig. 1). In the current the FE structural model, carbon atoms are treated as nodes in a mesh, and the C-C interactions are approximated with the use of 3D beam finite elements (B33 in Abaqus) with solid circular cross-section. For C-C bonds we have assumed the bond length
$a=0.142 \text{ nm}$, the effective bond diameter $t_b=0.34 \text{ nm}$, the bond stiffness $E_b=1000 \text{ GPa}$ and the bond Poisson ratio $\nu_b=0.3$. Because the nonlocal effects are mostly visible for short nanotubes [14], the (5,5) carbon nanotube having the length $L=2.83 \text{ nm}$ and average diameter $D=0.674 \text{ nm}$ was studied (Fig. 1).

![Figure 1. Structural FE model of single-walled carbon nanotube.](image)

As was mentioned in the introduction, the experimental observations have proved that vacancy defects are present in CNTs. The analysis of defective CNTs may have a significant influence on the explanation of how its existence deteriorate the mechanical behavior/properties of CNTs. To analyze the effect of small vacancy presence, we have constructed the defective structure – Fig. 2.

![Figure 2. FE model of carbon nanotubes: a) pristine and b) defective with one atom vacancy before reconstruction, c) defective after reconstruction (5- and 9-membered ring).](image)

From the pristine nanotube (Fig. 2a), one single carbon atom and three bonds were removed from the middle of CNT hexagon network to model a vacancy. Finally, a 12-membered ring appeared (Fig. 2b) with dangling bonds. The weakening of the structure is partially alleviated by the opportunity of nanotubes to cure defects in the atomic network by saturating dangling bonds. To do this, the 12-membered ring is reconstructed to 5- and 9-membered ring (Fig. 2c). The mechanical properties of pristine and defective CNTs in the static and dynamic regime were also previously studied by Muc and Chwał, see e.g. [3, 10, 17, 18, 19].

4. Results and discussion

4.1. Local and nonlocal Euler-Bernoulli model

The local and nonlocal Euler-Bernoulli beam models were used and the results for various nonlocal parameters were compared. For the circular nanobeam model of (5,5) CNT the following parameters were assumed: Young’s modulus $E=1000 \text{ GPa}$, Poisson’s ratio $\nu=0.3$, density $\rho=1200 \text{ kg/m}^3$, diameter $D=0.678 \text{ nm}$, and the length $L=2.83 \text{ nm}$. To consider the influence of nonlocal parameter on the free vibrations of CNT, we have used the nonlocal material parameter in the range $0\leq e_0\leq 10$ and
nondimensional length scale in the range $0 \leq e_0 a/L \leq 0.5$ assuming $a=0.142\text{nm}$. The applied values are comparable with other studies, e.g. [13, 20]. The results are presented in Fig. 3. The rise of the small scale parameter $e_0$ causes the lowering of eigenfrequencies. The decrease varies and depends on the mode number and boundary conditions. Fig. 4 shows how the length of CNTs deteriorates the eigenfrequencies for some representative results of C-F boundary conditions. Fig. 4 point out that the eigenfrequencies of short CNTs are very sensitive for mode number.

The higher sensitivity on the nonlocal parameter is observed for higher mode numbers what cases the faster dropping of eigenfrequencies (Fig. 5). Frequency ratio presents the ratio of nonlocal eigenfrequency to local eigenfrequency. The ratio is less than unity for all nonlocal parameters what suggests the local Euler-Bernoulli model overpredicts the eigenfrequencies for all modes. Comparing the local and nonlocal Euler-Bernoulli vibrational models, it is visible that the small scale parameter makes the structure more flexible (Fig. 5). The same observations for nonlocal plate models were presented, e.g. in [20]. In earlier paper of Chwał and Muc besides the free vibrations also the buckling of nanoplates was studied [6] based on our previous experiences [21,22,23].

4.2. Numerical results for pristine and defective carbon nanotubes

The eigenfrequencies for pristine and defective CNTs were analyzed involving the structural model. The results for various boundary conditions for the first three bending modes are listed in Table 1. It is visible that the eigenfrequencies of CNTs are also very sensitive to the boundary conditions. The
influence is much higher for low modes, whereas for higher modes the difference becomes less visible. To verify FEM results, a comparison of fundamental eigenfrequencies of short single-walled CNTs having small diameters with existing works has been made. The values from the current structural model of CNTs have been compared with resonant frequencies obtained by MD simulations and presented in the literature. We have focused on the CNTs with C-F boundary conditions. For C-F boundary conditions Hu et al. [24] for ratio $L/D=2.52$ obtained value 550GPa whereas Ansari et al. [25] for ratio $L/D=4.67$ achieved value 247GPa. The present FEM result for ratio $L/D=4.2$ is 373 GPa (see Table 1) what is in good agreement with the literature. The above comparison considers only FEM and MD because in this work we intended to propose the determination of the nonlocal parameter based on the structural FE model of the nanotube instead of commonly used MD simulations. However other methods are also applied in the dynamic analysis of CNTs, e.g. finite difference method (FDM) [26], boundary elements methods (BEM) [27], or differential quadrature method (DQM) [28].

### Table 1. Eigenfrequencies for pristine and defective CNT (5,5) [GHz].

| Mode no. | pristine CNT | defective CNT |
|----------|--------------|---------------|
|          | S-S | C-F | C-C | S-S | C-F | C-C |
| 1        | 1383 | 373 | 1814 | 1386 | 374 | 1808 |
| 2        | 3540 | 1818 | 3937 | 3501 | 1824 | 3914 |
| 3        | 5900 | 4084 | 5962 | 5750 | 4072 | 5807 |

The FE studies of free vibration of pristine and defective CNTs revealed deterioration. Generally, the slight decrease in eigenfrequencies of defective structures is observed however it varies for higher modes – see Table 1. It is worth to pointed out that even one carbon vacancy causes the modification in free vibrations between pristine and defective CNTs. It indicates that the higher number of defects in CNTs may have significant influence on their dynamic characteristic and should be taken into account when application of such carbon nanostructures is considered, e.g. in nanosystems design.

#### 4.3. Nonlocal parameter fitting

In general, the values generated from FEM are much lower than the values from the local beam models - see Table 1 and Fig. 3 for $e_0=0$. The local beam model overpredicts the eigenfrequencies for CNTs. It is particularly visible for higher modes. Here, the evaluation of $e_0$ is made for resonant frequencies because it is fundamental in CNT-based NEMS design. The fitting of the nonlocal material parameter $e_0$ is based on the comparison between local Euler-Bernoulli beam results with FE values of the structural model of pristine (5,5) CNT – Table 2.

### Table 2. Comparison of the FEM eigenfrequencies for pristine (5,5) CNT with the local and nonlocal Euler-Bernoulli model for variable and constant scale parameter $e_0$.

| Eigenfrequencies [GHz] | S-S | C-C | C-F |
|-----------------------|-----|-----|-----|
| FEM                   | 1383| 1813| 372 |
| Local Euler-Bernoulli beam | 1435| 3229| 511 |
| Nonlocal Euler-Bernoulli beam (variable $e_0$) | 1368 ($e_0=2$) | 1860 ($e_0=6$) | 372 ($e_0=10$) |
| Nonlocal Euler-Bernoulli beam (constant $e_0$) | 1127 ($e_0=5$) | 2085 ($e_0=5$) | 462 ($e_0=5$) |

Here, we show how the constant value of $e_0$ for all boundary conditions influence on resonant eigenfrequencies. According to our present calculations, the fitted nonlocal material parameter for resonant frequencies for all boundary conditions is equal to $e_0=5$ – Table 2. For the constant value of
the discrepancy between FEM and nonlocal beam results are present (e.g. for C-C about 15% and can be even higher for other boundary conditions and higher mode numbers). So, the calculation of the appropriate value of $e_0$ should be rather prepared separately for every boundary conditions – see Table 2. In the paper by Chwał [14] more detailed analysis is presented on variable $e_0$ versus boundary conditions.

5. Conclusions

The structural FE model has been applied in the description of free vibrations of CNTs and the results have been contrasted with the local beam model. The application of nonlocal beam models involves the analysis of small scale parameter which value depends on boundary conditions and mode number. The nonlocal scale parameters have been determined based on the nonlocal beam models fitting to FEM results. For short nanostructures, the influence of boundary conditions and the nonlocal parameter is highly visible. It was shown that the existence of defects in carbon nanotubes may influence the eigenfrequency value. However, the small vacancies in CNTs do not affect the eigenfrequencies significantly for all boundary conditions. The results presented here may be helpful in the design of very small-sized nanobeams applied in MEMs or NEMS where the size effect becomes significant.

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