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Investigation of the Free Longitudinal Vibration of Single-Walled Coiled Carbon Nanotubes Using Molecular Dynamics Simulation

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ABSTRACT: In this paper, the free longitudinal vibration of single-walled coiled carbon nanotubes with various boundary conditions is investigated via Molecular Dynamics simulation method. Heretofore vibration behavior of the single-walled coiled carbon nanotubes had not been studied with this technique, so using this method, longitudinal fundamental frequencies of single-walled coiled carbon nanotubes has been obtained by applying reactive empirical bond order potential without considering thermal effects. In order to perform a parametric study, the influence of the coiled carbon nanotubes diameter, the number of pitches and boundary conditions on the fundamental frequencies is evaluated. The results indicated that increasing the tubes diameter and the number of pitches (or length of coiled carbon nanotubes) lead to reducing the fundamental frequencies. Furthermore, the clamped-clamped single-walled coiled carbon nanotubes fundamental frequency is always higher than the cantilevered one. The results of this study can be used in vibration analysis of the nano-sensor and nano-actuator with coiled carbon nanotubes elements.

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1- Introduction

After the discovery of Carbon Nanotubes (CNTs) by Iijma in 1991 [1], these nanomaterials have been widely considered by researchers and scientists in the field of nanotechnology because of their extraordinary properties.

The Single-Walled Coiled Carbon Nanotubes (SWCCNTs) were theoretically predicted in 1993 by Ihara et al. [2], while the first observation of the Coiled Carbon Nanotubes (CCNTs) was possible in 2000 by Biró et al. [3] with a Scanning Tunneling Microscope (STM).

The CCNTs can be used as self-sensing mechanical resonators [4], in Nanoelectromechanical Systems (NEMS) [5], resonating elements, nano-actuators, nano-solenoids, nano-receivers, and non-volatile random access memory [6]. Another important application of the CCNTs is the reinforcement of composites [7].

In the vibrational analysis of the single-wall CCNTs, Fakhrabadi et al. [8] studied the vibrational behavior of CCNTs by molecular Mechanics-Based Finite Element Method (MMFEM) and determined their fundamental frequencies.

It is necessary to determine the values of the fundamental frequencies of the CCNTs for use in composite structures and(NEMS), nanosensors, and in particular in resonating elements. Hitherto, the vibrational behavior of the CCNTs has not been studied by molecular dynamics simulation. Therefore, in this paper, using the molecular dynamics simulation and Reactive Empirical Bond Order (REBO) potential, longitudinal vibrational behavior of these nanostructures will be studied under different boundary conditions. The effect of geometric parameters such as tube diameter and a number of pitches (or length of the CCNTs) as well as the effect of the boundary conditions will be investigated on the longitudinal fundamental frequency of the CCNTs.

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2- Methodology

2- 1- Modeling of the single-walled coiled carbon nanotubes

In this paper, modeling of single-walled coiled carbon nanotubes is performed using dual space approach [9] and coordinates of atoms of the CCNTs were extracted. In order to facilitate the comparison of the effect of CCNTs geometric parameters on the free vibration, as shown in Fig. 1 the three types CCNTs were modeled so that the inner diameter of the rings and the pitch length were approximately identical for all them.

2- 2- Simulation of vibration of the single-walled coiled carbon nanotubes

To study the free longitudinal vibration of CCNTs Molecular

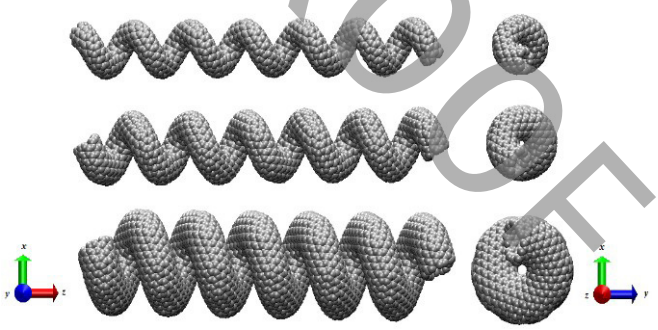

Figure 1. View of three types of the single-walled CCNTs.

Dynamics (MD) method is employed via the Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) open source software package.

The interaction of carbon atoms of the CCNTs is described by the second-generation REBO potential function [10]. A velocity-Verlet algorithm is used to integrate the equations of motion with a time step of 1 fs. After energy minimization step of the CCNTs by Conjugate Gradient (CG) algorithm, the system is relaxed for 30 ps under canonical Constant-Volume Ensemble (NVT ensemble) and Nosé-Hoover thermostat in a temperature 0.1 K to bring the CCNTs to the equilibrium condition. Then by microcanonical Microcanonical Ensemble (NVE ensemble) (adiabatic) vibration simulation is performed for the Clamped-Clamped (C-C), Clamped-Simply supported (C-S) and Clamped-Free (C-F) boundary conditions.

By applying initial excitation in the longitudinal direction the CCNTs is allowed to vibrate freely. The time history of the average longitudinal motions of the carbon atoms of the CCNTs is recorded every 100 steps as a time-domain response. Finally, the fundamental frequency is obtained using the Fast Fourier Transform (FFT) with the MATLAB software.

3- Discussion and Results

Free longitudinal vibration of the three types CCNTs are simulated under various boundary conditions. The effects of the tube diameter and number of pitches on the fundamental frequency are examined and the obtained results are presented in the following.

Fig. 2 shows the fundamental frequencies of the CCNTs under the Clamped-Clamped (C-C) boundary condition. By increasing the number of pitches, the longitudinal fundamental frequency of the CCNTs decreases. It is also observed that with the increasing the diameter of the tube, the longitudinal frequency of the CCNTs decreases. This result can be verified by transverse free vibration of the carbon nanotubes [11].

Fig. 3 shows the effect of different boundary conditions on the longitudinal fundamental frequency. As we can see, boundary conditions have a significant effect on the fundamental

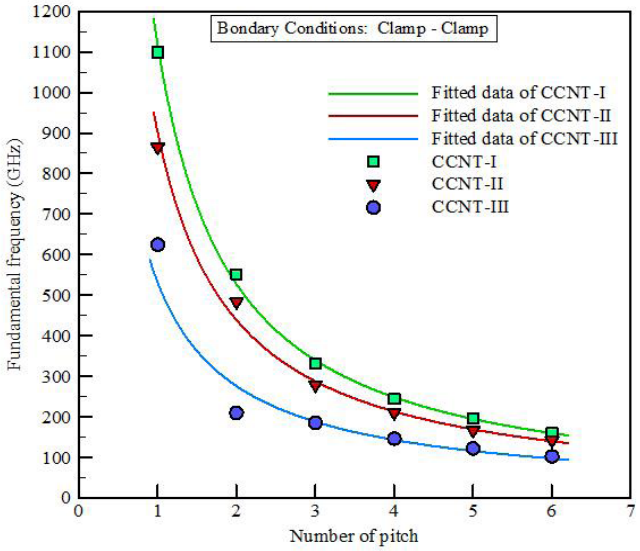

Figure 2. Fundamental longitudinal frequencies of the three types Clamped-Clamped single-walled CCNTs with a different number of pitches.

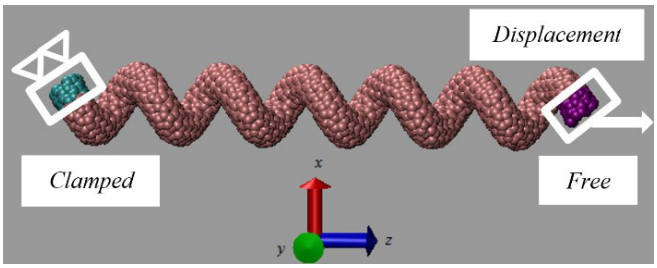

Figure 3. Comparison of fundamental frequencies resulted from present work with Fakharabadi et al [8].

frequency. In the Clamped-Clamped (C-C) boundary condition, the longitudinal frequency values of the CCNTs for the same diameter and number of pitches (up to 6 pitches) are always larger than the Clamped-Simply supported (C-S) and Clamped-Free (C-F) boundary conditions.

Prior to this study, only Fakhrabadi et al. [8] studied the vibration of the CCNTs by MMFEM under different boundary conditions. Fig. 3 also shows the comparison of the results of the present study with the results of reference [8].

4- Conclusions

In this paper, the free longitudinal vibration of three types of the CCNTs with various diameters and number of pitches under Clamped-Clamped (C-C), Clamped-Supported (C-S) and Clamped-Free (C-F) boundary conditions investigated via molecular dynamics simulation method. The results indicated that the longitudinal fundamental frequency decreases with increasing tube diameter and number of pitches. Furthermore, the Clamped–Clamped SWCCNT's fundamental frequency is always higher than Clamped-Simply Supported (C-S) and Clamped-Free (C-F) one.

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