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Modal analysis of multi-walled carbon nanocones using molecular dynamics simulation

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ABSTRACT

To design carbon nanocone-based sensing and actuating nanodevices, it is necessary to study their vibrational behavior. For this purpose, modal analysis of multi-walled carbon nanocones are performed using molecular dynamics simulation. Initial closed-tip atomic structures of the carbon nanocones with different apex angles are modeled through a proposed method which is based on the molecular dynamics simulation. The dependency of the resonant frequencies and their corresponding three-dimensional mode shapes on different geometric parameters of multi-walled carbon nanocones are investigated. The results indicate that the order of mode shapes is influenced by the number of layers and apex angle of the multi-walled carbon nanocones. The results also show that the variation of the resonant frequencies with the number of layers depends on the apex angle and shape of the modal displacement. The vibrational behavior of the multi-walled carbon nanocones is also compared with that of the multi-walled carbon nanotubes.

1. Introduction

In modern industry, carbon nanostructures are of great interest because of their potential for structural and electronic applications taking advantage of their novel properties. In particular, cylindrical and conical morphologies of carbon nanostructures are pioneer in this type of applications due to their large surface area and unique shape. Since the discovery of carbon nanotubes (CNTs) [1] and carbon nanocones (CNCs) [2], there has been a great deal of experimental and theoretical researches that focused on their characterization. CNTs and CNCs are good candidates as sensing and actuating elements in nanoscale devices [3–9]. Among these applications, their usage as atomic force microscopy (AFM) tips [3,8] is of particular interest. The proper implementation of CNTs and CNCs as AFM tips, requires comprehensive understanding of their dynamic behavior and a remarkable amount of studies have been performed to investigate the vibrational behavior of these two nanostructures [10–32]. However, the reported works in this field for CNCs are relatively limited as compared with CNTs. Also, the inherent thermal vibration of CNT-based AFM tips, due to the high aspect ratio and small diameter of the nanostructure, reduces imaging quality, but, the sharp tip and less flexibility of CNCs, make them a better candidate to be used as AFM tips [8,33]. So, precise characterization of CNCs is of great importance considering all aspects of this nanostructure.

Duo to the technical difficulties associated with the experimental methods for investigating the structures at nanoscale, theoretical and numerical approaches are usually preferred. Continuum mechanics models, molecular mechanics method and molecular dynamics (MD) simulation have been widely used to study and approximate the behaviors of the nanostructures. In the first approach, which is usually based on the nonlocal elasticity theory, CNCs are modeled as beams with varying cross sections [21,30] or as shells [22–24]. The molecular mechanics method is a combination of continuum mechanics models and atomistic approaches. In this method, the bonds between different atoms are represented by structural elements, whereas, the atoms are considered as mass elements and the material constants of the structural elements are obtained by equating the energies of the molecular and structural models. In this way, the nanostructure can be treated as a frame structure and its modal analysis can be performed using the standard finite element method. The vibrational behavior of CNCs, based on this method, has been studied in Refs. [26–28,31].

In the third approach, i.e., MD simulation technique, the interaction between different atoms is described by some potential energy functions and the displacement gradient of these functions results in the applied forces on each atom. Then, these forces are used in Newton's second law to determine the movement of each atom. This method can provide a detailed understanding about dif-

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ferent behaviors of a discrete structure at the nanoscale by taking into account all the effective parameters. The main drawback of this technique is its high computational cost, in comparison with the two other approaches. Aside from being computationally expensive, MD simulations always involve some inevitable errors as a result of their numerical nature and some basic concepts such as cut-off radius, etc. However, MD simulations have some advantages over continuum mechanics models and molecular mechanics method. The main advantage may be its capability in providing direct control over the temperature of the nanostructure. The other advantage of this method is that material properties such as Young's modulus and Poisson's ratio are not needed to study the vibrational characteristics of the nanostructures; while, the accuracy of the results obtained using continuum mechanics models depends strongly on such material properties. These material parameters for CNTs and CNCs are proven to be size dependent [34,35] and there is a big scattering in the experimentally reported data. In addition to the material constants, wall thickness of CNTs and CNCs is not a well-defined quantity, which is required in continuum mechanics models. On the other hand, in the molecular mechanics method, the simple harmonic form is usually adopted to describe the energy of bonded interactions under the assumption of small deformation, and also, the nonbonded van der Waals (vdW) interactions are usually neglected. While, in general, MD simulation approach can describe both bonded and nonbonded interactions in a more realistic nonlinear way through different appropriate potential functions. There are a limited number of studies which have utilized MD simulation to investigate the vibrational behavior of CNCs. Firouz-Abadi et al. [29] examined the effect of geometric parameters and temperature on the resonant frequencies of cantilever CNCs using MD simulation. Their results indicate that the resonant frequencies are approximately insensitive to the temperature. Using MD simulation and continuum mechanics beam model, Hu et al. [30] investigated the free transverse vibration of cantilever CNCs and showed that the fundamental frequency of a CNC is higher than an equivalent CNT which has the same length and top radius as CNC. Ansari et al. [31] conducted molecular mechanics and MD simulation methods to study the vibration of CNCs with different lengths, apex angles, and boundary conditions. They proved that the effect of boundary conditions on the natural frequencies is more prominent for CNCs with smaller apex angles. In most of the MD-based vibrational studies, including the ones mentioned above, the desired resonant frequencies of the nanostructures are obtained by applying proper initial deflections similar to the desired mode shapes. This method demands several MD simulations to determine the resonant frequencies of different mode shapes. However, thermal oscillations of atoms during MD simulation of a nanostructure can be used to extract resonant information [20]. Based on this fact, a method was developed in [32] to extract the resonant frequencies and corresponding three-dimensional mode shapes of CNCs using only one MD simulation without imposing any initial deflection on the nanostructure. The effect of the length, apex angle, and boundary conditions on the resonant frequencies and the order of modal displacements were investigated and the results showed that the transverse, torsional, and longitudinal mode shapes shift toward higher mode numbers as the length or apex angle increases. Although, the proposed method was used for CNCs, it can be applied to other types of nanostructures.

CNTs and CNCs can be structurally categorized as single-walled or multi-walled and open-tip or closed-tip nanostructures. Topologically, pentagonal defects are needed to be introduced in the hexagonal graphitic network of CNTs and CNCs in order to close their tip. Depending on the number of pentagons at the apex, from one to five, there are five possible CNCs with cone angles of 112.9°, 83.6°, 60°, 38.9°, and 19.2° [36]. A CNT can be regarded as a CNC with apex angle of 0° and six pentagonal rings. In general, most laboratory-grown CNCs are multi-walled carbon nanocones (MWCNCs) with closed tips. The only single-walled carbon nanocone (SWCNC) that has been produced in large quantities, can be found in particles named carbon nanohorns which are composed of an aggregate of many SWCNCs with apex angle of 19.2° [37].

In fact, modeling of the closed-tip atomic structures of SWCNCs is not simple. However, in this study, a method has been proposed to construct these closed-tip nanostructures with true arrangement of pentagonal defects based on MD simulation. Upon generating the tip models, atomic structures of MWCNCs with any given length can be obtained using a simple algorithm. Although, the vibrational behavior of the generated nanostructures has been investigated in the present work, however, they can be used in analyzing their other properties.

To the best of the authors' knowledge, only the vibrational behavior of open-tip SWCNCs has been theoretically reported before [21–32]. Therefore, investigating the vibrational behavior of closed-tip MWCNCs, which are more common in practice than open-tip SWCNCs, can provide useful information in designing CNC-based nanodevices. Hence, this work aims to perform three-dimensional modal analysis of closed-tip MWCNCs using MD simulation and to compare them with the multi-walled carbon nanotubes (MWCNTs). In the following sections, after modeling the

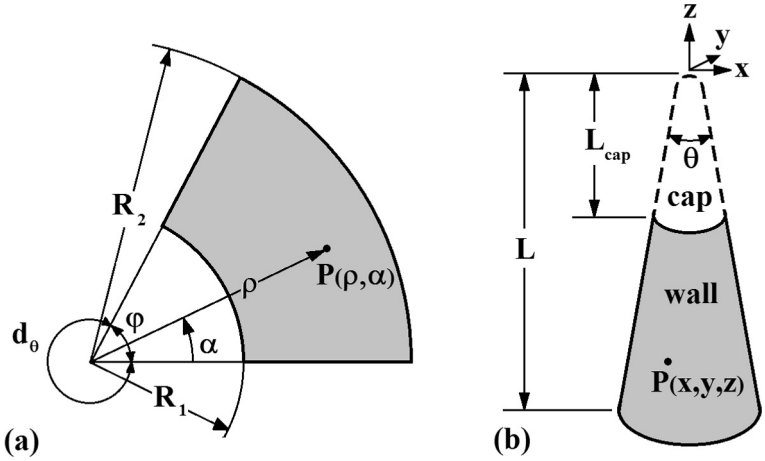

Fig. 1. Symbols and variables used in the transformation from (a) the polar coordinates of the atoms in the plane of the graphene sheet to (b) their Cartesian coordinates in the constructed SWCNC.