Computational Materials Science 115 (2016) 72–76

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Energy absorption induced oscillation of a rotating curved carbon nanotube in a nano bearing

Zhaoliang Gao [a], Haifang Cai [b], Jing Wan [b], Kun Cai [b,c,*]

[a] Institute of Soil and Water Conservation, Northwest A&F University, Yangling 712100, China
[b] College of Water Resources and Architectural Engineering, Northwest A&F University, Yangling 712100, China
[c] Research School of Engineering, The Australian National University, Canberra, ACT 2601, Australia

ARTICLE INFO

Article history:
Received 15 November 2015
Received in revised form 12 December 2015
Accepted 17 December 2015
Available online 2 February 2016

Keywords:
Nano device
Carbon nanotube
Curved tube
Transmission system
Resonance

ABSTRACT

In a nano bearing, a curved inner carbon nano tube (CNT) constrained by two short outer CNTs will have an oscillation along the curved axis of the tube when a specified rotational velocity is input on one end of the inner tube. It is found that the free end has periodic axial translational oscillation and the amplitude of oscillation is very high when the frequency of the input rotational velocity is close to an eigen/resonance frequency of the system, i.e., energy absorption of the inner tube from the interaction between the inner and outer tubes. Higher curvature of the inner tube leads to higher value of fundamental frequency of the system. The free end of the inner tube also has obvious torque oscillation. Both of the axial translational oscillation and torque oscillation of the free end can be used as output signals of the system as working in a nano signal generator. The mid part of the inner tube, i.e., the part between two outer tubes, has obvious in-plane vibration, which indicates that the present nano bearing is a two-dimensional device.

1. Introduction

With the decreasing of the sizes of components in a micro-electro-mechanical system (MEMS), both of theoretical study and development of experiment techniques on design of a nano-electro-mechanical system (NEMS) become urgent in recent years. Due to excellent physical properties, carbon nano structures, e.g., carbon nanotube (CNT) [1–3], graphene sheet [4,5], carbon nanoscroll [6,7], etc., attract much attention in the studies. In particular, CNT-based oscillator/bearing/motor is one of the new conceptual designs of NEMS.

By experiments on axial tension of inner tube in multi-walled carbon nanotubes (MWCNTs), Cumings and Zettl [2] test the inter-shell friction force and find that the extruded core can be retracted inside the outer tubes quickly when the core is released. They explain that the van der Waals force drives the retraction, and demonstrate a possible path to construct a gigahertz-frequency oscillator. Zheng and Jiang [8] propose the mechanical model of such nano oscillator. Following the finding, a series of investigations have been made to give a design of the nano device. For example, Legoas et al. [9] research the stability of the nano oscillator with molecular dynamics (MD) simulations.

Many experimentalists try to fabric such nano device [2,10–12]. However, up to now, there is no one nano device with size of only few nanometers. The reason is that the energy dissipation is serious during relative motion between adjacent tubes and a long-time stable motion cannot be easily maintained. Using MD simulations, Zhao et al. [13] imply that the friction phenomenon between two adjacent CNTs is the major reason for the transmission of orderly translational kinetic energy into disorderly thermal vibrational energy. As can be seen, the damping behavior still exists even in short-tube oscillators (see Fig. 1c in Ref. [13]). Guo et al. [14] compare the energy dissipation rates between commensurate and incommensurate double-walled CNT (DWCNT)-based oscillators. Their results show that the inter-tube friction is proportional to energy dissipation rate, but inversely proportional to the oscillation frequency. In a long-tube oscillator, the damping oscillation is very clear [15]. Cook et al. [16] find that friction within a rotating CNT bearing is proportional to relative rotating speed and system temperature, but slightly depends on the length and mean diameter of inner tube. Hence, to obtain a nano oscillator/motor with controllable amplitude or frequency, the energy dissipation due to inter-tube friction should be made up by absorbing energy from environment. For example, Neild et al. [17] suggest to using periodic forces to excite the oscillation meeting the conditions of controllability. Kang et al. [18] try to find a frequency-controlled CNT-based oscillator, which is made from three co-axial CNTs,

* Corresponding author at: Research School of Engineering, The Australian National University, Canberra, ACT 2601, Australia

E-mail address: kuncai99@163.com (K. Cai).

http://dx.doi.org/10.1016/j.commatsci.2015.12.028
0927-0256/

i.e., two outer tubes and one inner tube. By adjusting the gap between two outer tubes, the oscillation of the inner tube behaves differently. Either external electricity field or non-uniform heating method can also be adopted to drive a nano rotary/linear motor. For example, Fennimore et al. [10] choose the MWCNTs as a key motion-enabling component in a nano electricity-driven actuator. Bourlon et al. [11] attach a plate on the MWCNTs-based bearing, which is driven to rotate by a charged stator. By experiments, Barreiro et al. [12] find the axial motion of a cargo on a movable CNT relative to another coaxial CNT with axial thermal gradient. Further study on thermal-gradient driven motion is given by other researchers [19–22]. Peculiarly, Cai et al. [23] find that the uniform temperature field can also drive the rotation of a DWCNTs-based motor.

From the forgoing review, few work demonstrates the oscillation and simultaneous rotation of the movable component in a nano motor. Recently, Cai et al. [24] find that the high-speed rotating inner tube in a fixed outer tube can be excited to oscillate periodically. The mechanism is that the rotational kinetic energy of inner tube becomes into both of thermal vibration energy of system and axial translational kinetic energy of inner tube. This finding indicates that a stable oscillation can also be obtained when the inner tube has a stable rotational speed.

Different from both of the work by Kang et al. [18] and Cai et al. [23], in the present study, we propose a new rotation–oscillation transmission system from DWCNTs. But in the present model, the inner tube is curved [25–32] and constrained in two short outer tubes. Giving a specified rotational speed on one end of the inner tube, the other tube end has different dynamic response. MD simulations are carried out to show the dynamic response.

2. Models and methods

Three models for the system shown in Fig. 1b–d are considered: Model 1: curvature radius of $R = 5.161$ nm when $n = 128$; Model 2: $R = 8.019$ nm when $n = 164$; and Model 3: $R = 11.194$ nm when $n = 204$.

The molecular dynamic (MD) simulation is carried out using LAMMPS [33]. In simulation, the AIREBO potential [34] is adopted to indicate the interaction of the carbon atoms in system. The time integral increment is 1 fs. Before simulation, 400 ps of Nosé–Hoover bath at canonical (NVT) ensemble with $T = 300$ K is applied on the system for relaxation. During relaxation, the top 4 layers of the upper right end of the inner tube are fixed. The two outer tubes are fixed, too. After relaxation, the input rotational frequency is applied on the lower left end of the curved inner tube, and the value of gap, output rotational frequency and the potential of inner tube are output.

To find the influence of the input rotational frequency of the inner tube on the dynamic response of system, the value of ω_{in}, is set to be 20, 50, 80, 120 and 150 GHz, respectively.

3. Results and discussions

From either *potential history* curve or *output rotation history* curve in Table 1, one can find that the system tends to be stable after ~2 ns. The wild fluctuation of the output signals of system in the initial stage is mainly due to the sudden application of the input rotation of the curved inner tube. After 2 ns, most of the output signals keep stable. Two characters of the output signals are necessary to be demonstrated. One is the damping behavior. The other is the stable large amplitude vibration of the upper right end of the curved inner tube.

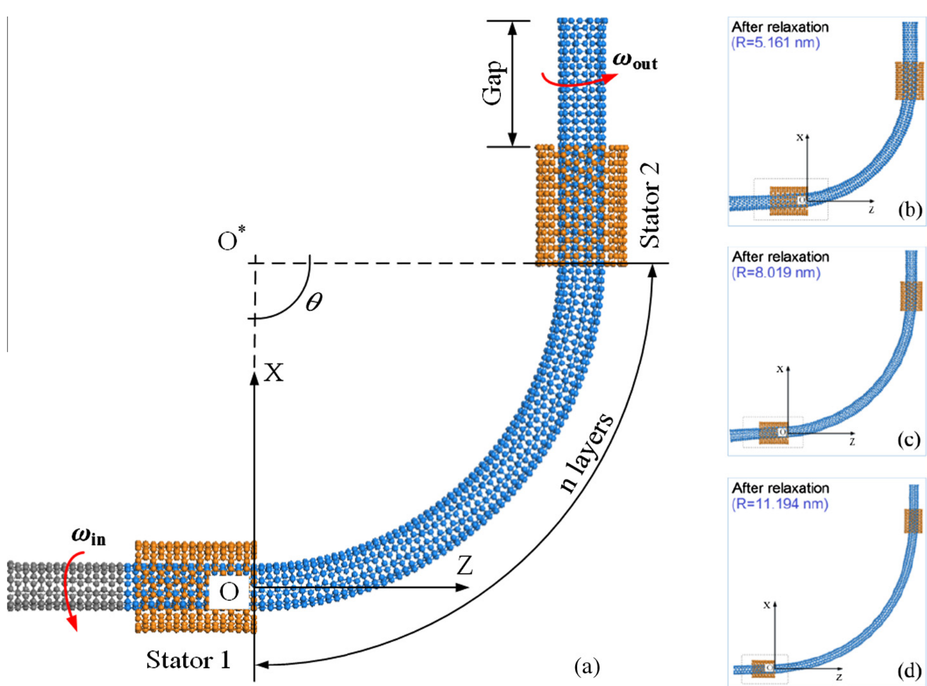

Fig. 1. (a) The initial simulation model for a nano rotation–oscillation transmission system, in which the two straight 16-layer outer (10, 10) carbon tubes (orange parts) are fixed. Initially, there are 16 layers of atoms on each end of the inner tube beyond the constraint of the stators. The lower left end (grey part, 16-layer) of the curved inner (5, 5) carbon nanotube has a constant input rotational speed, i.e., ω_{in}, and the upper right end has an output rotational frequency, i.e., ω_{out}. The value of gap is the axial distance between the upper right end of the inner tube and stator 2. Between the two outer tubes, the mid part of the inner tube with n layers is curved. And the radius of the curved axis, i.e., R, is the distance between O and O*. θ is the central angle, and equal 90° in this study. After relaxation (b, c and d), near stator 1, the inner tubes do not keep co-axial with the outer tubes and the included angle is ~2° (see the sections within dashed boxes). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)