

Vibrational analysis of carbon nanotubes in thermal environments

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Abstract

Based on molecular dynamics (MD) simulations, the properties of free transverse vibrations for single-walled and double-walled carbon nanotubes (CNTs) are studied in thermal environments. The computations are carried out for two types of armchair single-walled carbon nanotubes (SWCNTs) with different lengths, and results are also compared between certain double-walled carbon nanotube (DWCNT) and its constituent SWCNT. It is shown that the corresponding natural frequencies of nanotubes depend strongly on their geometries. While temperature changes only have small effects on transverse vibration properties. The results demonstrate that adding inner nanotubes to the outer one will decrease the natural frequencies.

Carbon nanotubes have received considerable attention since they were reported in 1991. Lately a lot of research has been devoted to the vibrational characteristics of CNTs [1-9]. In these researches, elastic continuum model have been widely used [1-5]. However, the significant scatterings are found in their numerical results because different effective mechanical properties of nanotubes were applied in the continuum model, which affect strongly the applicability of elastic theory [10]. On the other hand, a great deal of research indicates that the mechanical properties of CNTs are related to temperature changes [11-13], while theoretical investigations of thermal effect on vibrations of CNTs are very limited.

In this paper, the properties of free transverse vibrations for SWCNTs and DWCNTs are systematically studied by employing MD simulations. The temperature changes from 300K to 1200K are taken into account. The predicted results of DWCNTs are compared with those of their constituent SWCNTs. The effects of nanotube radius and length on natural frequencies of CNTs are carefully investigated.

The numerical simulations in this paper are carried out by using the MD method. We employ Brenner's "second generation" REBO potential [14] to describe the short-range covalent C-C interactions. The long-range van der Waals interaction is modeled by the much

applied Lennard-Jones 12-6 potential [15]. In the MD simulations, heat conduction and temperature conversion are accomplished via the Nose-Hoover feedback thermostat [16].

In the MD simulation of free transverse vibrations, both ends of each tube are held rigid so that the atoms of the end are constrained to deform as a whole. One end of the CNT is kept fixed, while the other rigid end is only allowed to move in axial direction.

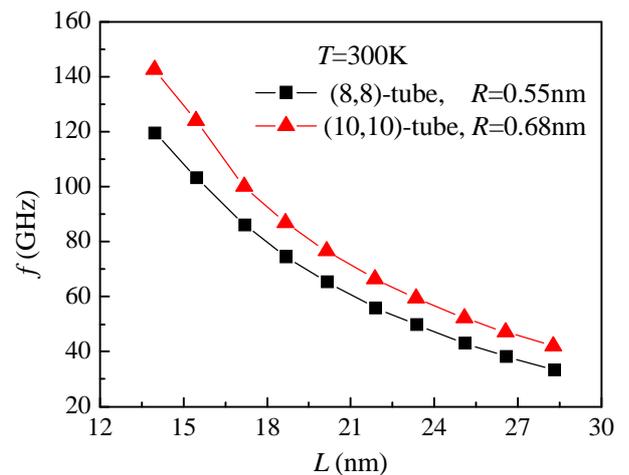


Fig. 1 Effect of nanotube size on the natural frequencies of SWCNTs at 300K.

We first examine the vibration properties of SWCNTs at the room temperature of 300 K. Two pairs of armchair nanotubes are selected. The armchair (8,8) SWCNTs

with radius of 0.55 nm and lengths varying from 13.98 nm to 28.34 nm, as well as armchair (10,10)-tubes having radius of 0.68 nm and lengths varying within the same range. The effects of nanotube length and radius on the natural frequency are depicted in Fig. 1, in which f is the natural frequency with vibrational mode being a half-sine shape, and L is the nanotube length. It can be seen that the frequency f decreases when nanotube length increases, and the relationship is nonlinear for both CNTs. For the same length of SWCNTs, the value of f for (10,10)-tubes is larger than that for (8,8)-tube with relatively smaller radius. Molecular mechanics studies by Georgantzinos *et al* [7] as well as finite element investigations of Mir *et al* [8] gave the same conclusions.

Table 1 Comparisons of the natural frequencies (GHz) between (9,9,116) SWCNT and [(4,4) (9,9) 116] DWCNT at different temperature.

Nanotubes	300K	700K	1200K
(9,9,116) SWCNT	38.30	38.62	38.79
[(4,4) (9,9) 116] DWCNT	33.19	34.01	34.19

To investigate thermal effects, we select a DWCNT and one of its constituent SWCNT. The armchair (9,9)-tube having radius of 0.61 nm and length being 28.23 nm, as well as the armchair [(4,4) (9,9)] DWCNT having inner and outer radii being 0.45 and 0.61 nm respectively and very close length with the single-walled one. The present MD simulations reveal that the inner and outer tubes of DWCNT can deform accordantly during vibration process due to van der Waals interaction between walls. Table 1 shows the corresponding natural frequency f with vibrational mode being a half-sine shape at 300K, 700K and 1200 K. It is seen that rise in temperature leads to increases of frequency, while the increment is small. With the temperature increasing from 300 K to 1200 K, the enhancements of predicted natural frequency are 1.27 % for the (9,9)-tube and 3.00 % for the DWCNT. The vibrations behavior of DWCNTs depends even stronger on temperature changes than that of its constituent SWCNTs do. To explain this, the DWCNTs will suffer greater thermal

effects with more violent oscillation of all surface atoms as temperature rises than SWCNTs behave. Table 1 also shows that the natural frequency of (9,9)-tube is larger than that of [(4,4) (9,9)] DWCNT, which demonstrates that adding inner nanotubes to the outer one will decrease the natural frequencies.

MD simulations show that the vibrational mode of CNTs presents as a half-sine shape, which is in accordance with the first mode of bending vibration for SWCNTs in reference [7]. We found the mode shapes are similar at different temperature otherwise more local geometric imperfections in the tubes at higher temperature due to wider thermal oscillation of atoms.

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