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Carbon nanotube oscillators: Effect of small bending strain

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ABSTRACT

The oscillatory behavior of CNT oscillators, initially subjected to bending, is studied under constant temperature using molecular dynamics simulations. We constrain the rotational motion of the inner CNT by imposing a small bending deformation to the initial structure. Our observation suggests that this constraint does not enhance the oscillation stability of CNT oscillators. However, oscillations of the shorter inner CNT are severely affected by the bending strain. As the curvature increases, the stability reduces significantly, resulting in faster damping of oscillations. The exchange of energy from orderly translational motion of inner CNT to high frequency modes of outer CNT is also observed.

Keywords: Carbon nanotube, bending, oscillator, molecular dynamics

1. INTRODUCTION

Carbon Nanotubes (CNTs) are well known for their outstanding mechanical, electrical and thermal properties, and there is a growing interest in the development of CNT-based mechanical systems. Recently, fabrication of CNT-based oscillators has been realized by Cumings and Zettl[1] who observed extremely low friction oscillations between the walls of multiwalled-CNTs. CNT oscillators have been proposed in various applications viz. actuators, surface profiling devices, non-volatile memory devices, and inertial measurement systems. These oscillators may be subjected to some sag during operation, which could affect the oscillation behavior considerably. A few recent experimental[2] and many simulation studies[3-7] has been carried out to study the behavior of CNT oscillator. The influence of various imperfections in the form of topological defects on the outer CNT has also been addressed [5, 7, 8].

The effect of single S-W defect (grooving) on the oscillatory behavior of double-walled CNT oscillators was studied by Wang et al.[7] using molecular dynamics simulations. A significant reduction in oscillation energy leakage was observed in their results. The presence of a defect on the outer CNT causes a grooving effect on oscillatory motion by constraining the rotational freedom, which in turn reduces the frictional effects between the sliding CNTs. They also showed that the effect of grooving reduces as the temperature increases.

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In the present work, we constrain the rotational motion of the inner CNT by imposing a small bending deformation to the initial structure. The oscillatory behavior of CNT oscillators initially subjected to bending deformation is investigated under constant temperature using molecular dynamics simulations.

2. MODELLING AND SIMULATION

This section describes the procedure for preparing the initial bent configurations of DWCNTs to observe the oscillatory behavior of inner CNT. The MD simulations were conducted using in-house FORTRAN code. The interactions among Carbon atoms within the CNTs are described by modified Morse potential[9] which has been successfully used to study the mechanical properties of CNTs[10, 11] and the interactions between walls CNTs are described by Lennard-Jones potential. Figure 1 illustrates the atomic structure of double-walled CNT-based oscillator considered in our study which is at the start of oscillation. The DWCNT of 9.6 nm long is considered for the study which is comprised of (10,10) and (5,5) CNTs. Initially the whole system is relaxed for 50 ps, and then CNT is deformed to a specified curvature, followed by 500 ps of simulations of oscillations. Berendsen thermostat scheme[12] applied to maintain system temperature constant at 1K. Velocity Verlet integration scheme is used to solve the Newton's equations of motion and a time step of 1fs is used for all the simulations.

Atoms of two rings near both ends of the outer CNT are defined as boundary atoms. Bending deformation was achieved by displacing the boundary atoms with a steady increment of bending angle by applying a global curvature of 10^{-5} nm^{-1} until an end curvature is reached. After each increment of bending angle, the whole system is relaxed for 200 steps by constraining the boundary atoms.

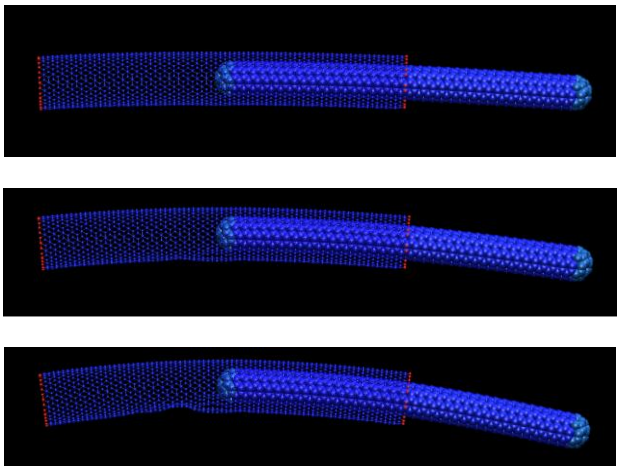

Figure 1. Snapshots from the molecular dynamics simulations depicting oscillatory behavior of a (5,5) CNT inside of a (10,10) CNT with initial bending curvatures of $0.01nm^{-1}$, $0.02nm^{-1}$, $0.03nm^{-1}$(top to bottom in the panel)

3. RESULTS AND DISCUSSION

CNT oscillator composed of DWCNT having initially subjected to bending deformation is studied using MD simulations. As mentioned before, the main objective was to investigate the effect of initial bending deformation of total structure on the oscillation stability. We studied the oscillation characteristics at three different curvatures (0.001 $Å^{-1}$, 0.002 $Å^{-1}$, 0.003 $Å^{-1}$) and at three different inner tube lengths (95Å, 55Å, 18Å) as presented in Figure 2. Rotational motion of the oscillating inner tube is constrained by the initial bending. No advantage of oscillation stability is found with this rotational constrain; the significantly small amount of rotational energy in comparison to the translation motion in such a deformed structure might be the reason.

We found that oscillation stability depends on curvature of oscillator and length of inner tube. As the curvature of oscillator increases, for a fixed inner tube length, stability decreases and frequency increase is very small. For a fixed inner tube length, increased curvature damps the oscillations quickly and for fixed curvature, increased inner tube length increases the stability of oscillations.

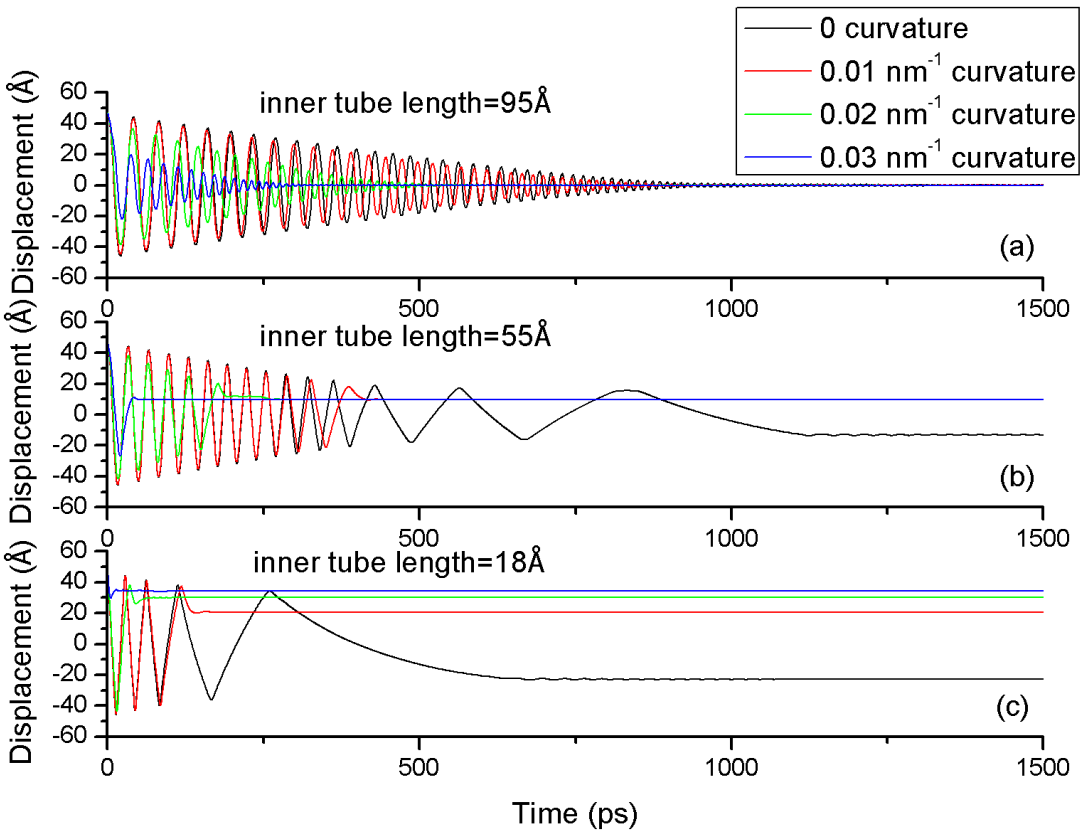

Figure 2 Oscillation profiles for different oscillating inner CNT lengths (a) 95 Å (b) 55 Å (c) 18 Å. For all the cases, the length of outer (10,10) is 9.6 nm, and the extrusion distance is 4.8 nm.

Further, to analyze the damping mechanism of the oscillations due to the imposed bending strain, along with monitoring the resultant vdW force and energy we also computed the phonon kinetic energy, i.e., the relative kinetic energy of the two CNTs, which can be written as[13]:

$$K_{rel}(t) = \sum_i \tfrac{1}{2} m_i \left| v_i^{in} - v_{ave}^{in} \right|^2 + \sum_j \tfrac{1}{2} m_j \left| v_j^{out} - v_{ave}^{out} \right|^2 \quad (1)$$

where v_i^{in} (v_j^{out}) and m_i (m_j) are the velocity and the mass of the i^{th} (j^{th}) atoms in the inner (outer) tubes, respectively; v_{ave}^{in} (v_{ave}^{out}) is the average velocity of atoms in the inner (outer) tube. The relative kinetic energy is a measure of phonon energy transfer from orderly translation motion of inner CNT to outer CNT. As suggested in Ref. [13], the relative kinetic energy provides an accurate estimate of the dynamics of kinetic energy transfer among the two CNTs.

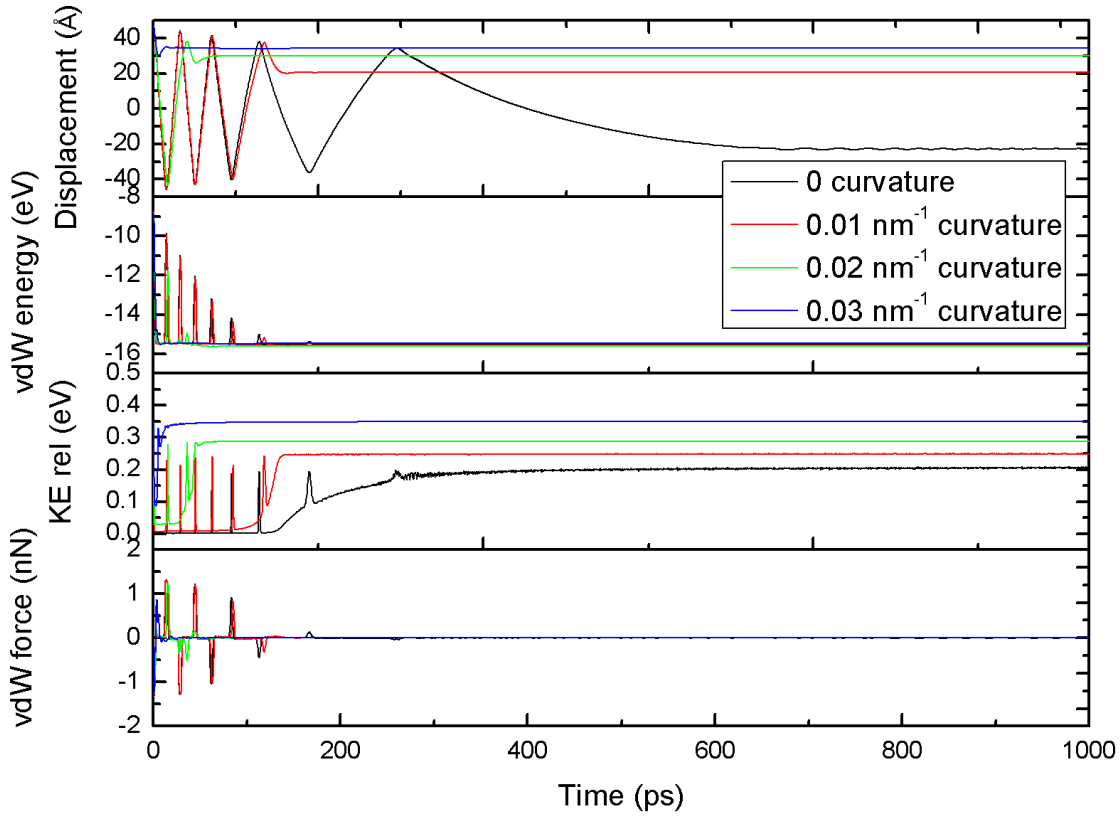

Figure 3 Oscillatory behavior of 18 Å long inner CNT at three different bending strains. Panels top to bottom: Displacement of inner CNT with time, vdW energy with time, relative kinetic energy with time and the resultant vdW force with time.

Figure 3 to 5 shows the detailed time evolution of these properties corresponding to the displacement of the inner CNT. The fluctuations in vdW energy is quickly coming to disappear as the curvature increases. These fluctuations or corresponding oscillatory vdW force are indicating the oscillating motion of inner CNT. Thus the increasing curvature hinders the oscillations quickly. The quick rise of relative kinetic energy in 0.03 nm^{-1} curvature than other low curvatures indicates the early transfer of orderly kinetic energy of inner CNT to the outer CNT. In the case of 95Å inner CNT (Figure 5) the clear monotonic trend of decaying oscillations with increasing curvature is shown. We can observe the constant exchange of kinetic energy through out the oscillations except at the end as indicated by the constant rise in the relative kinetic energy which is due to the fact that the simulations are conducted at 1K. The absence of thermal effects at 1K makes the smooth oscillations possible. However the vdW energy and resultant force on the inner CNT gradually decaying which eventually lead the inner CNT to reach stationary state.

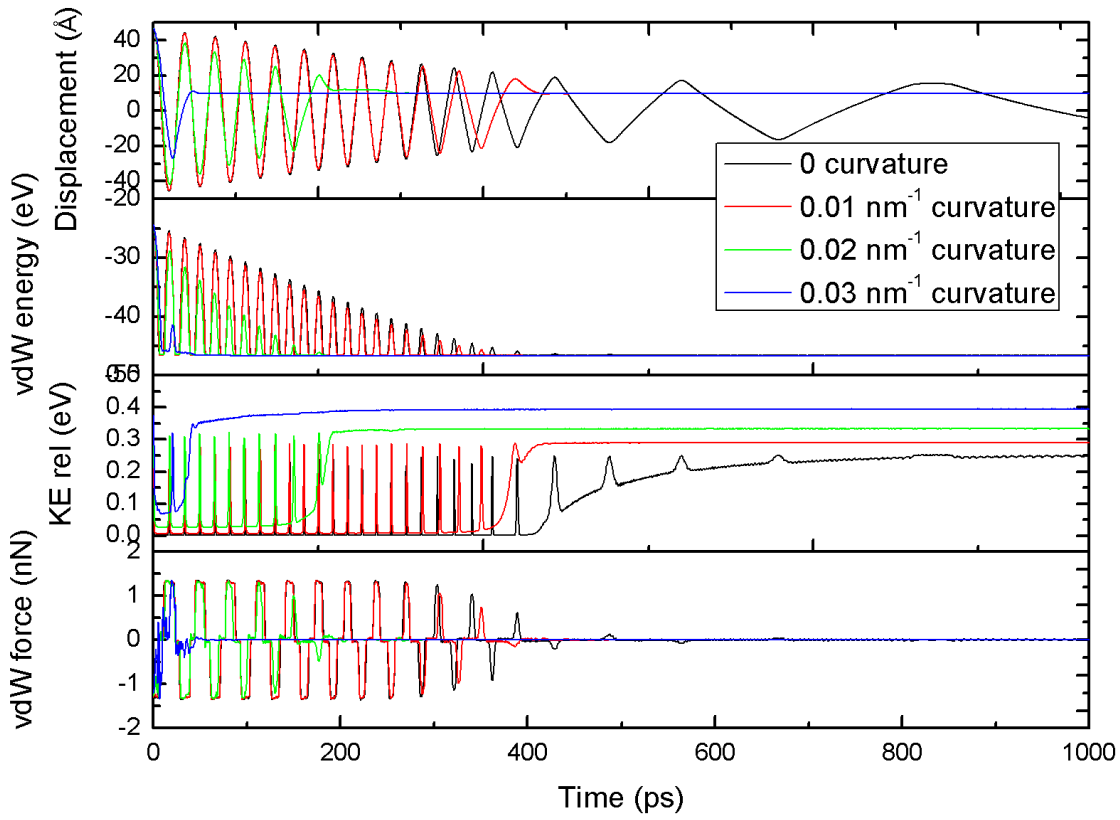

Figure 4 Oscillatory behavior of 55 Å long inner CNT at three different bending strains. Panels top to bottom: Displacement of inner CNT with time, vdW energy with time, relative kinetic energy with time and the resultant vdW force with time.

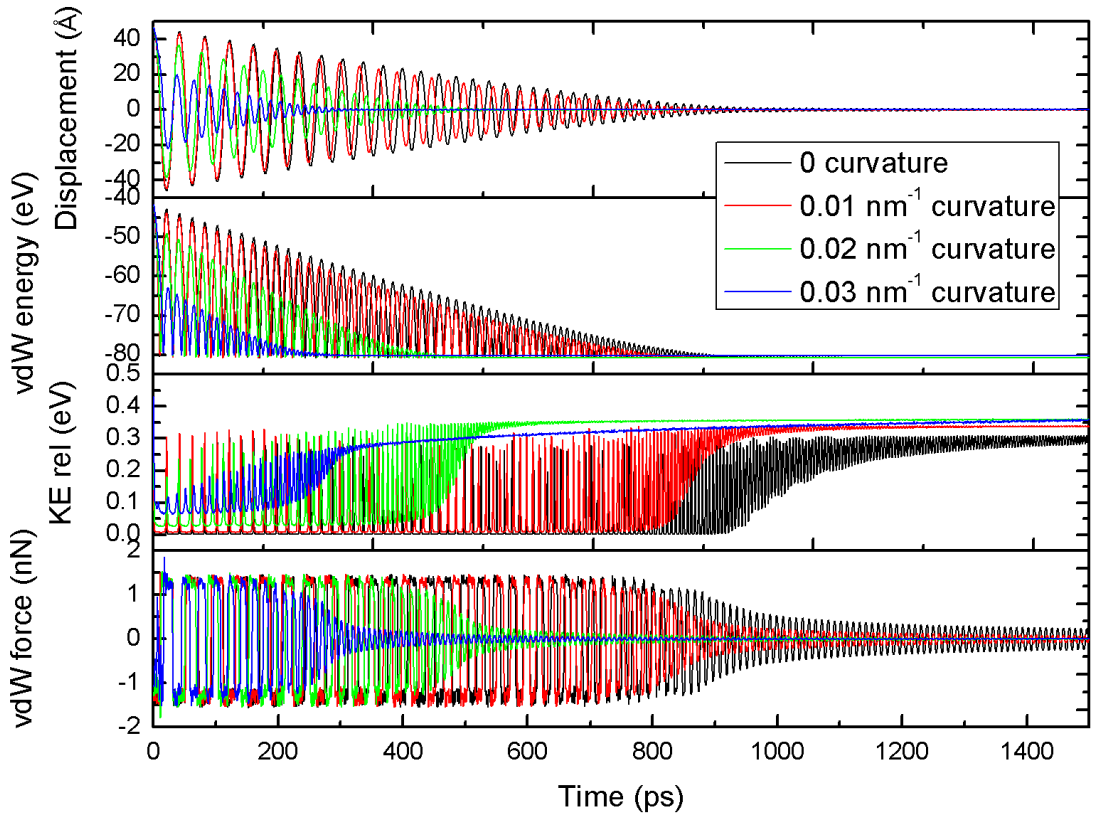

Figure 5 Oscillatory behavior of 95 Å long inner CNT at three different bending strains. Panels top to bottom: Displacement of inner CNT with time, vdW energy with time, relative kinetic energy with time and the resultant vdW force with time.

4. CONCLUSIONS

In summary, employing a set of MD simulations at temperature of 1 K, we have shown in detail the oscillatory behavior of CNT oscillators subjected to an initial bending strain. We found that the increasing curvature hinders the oscillations quickly. The curvature effect is more pronounced in case of shorter inner CNT. Initial bending deformation constrained the rotational motion of inner CNT, however this constraint is not enhancing the stability of oscillations. Using the relative kinetic energy, we observed the exchange of energy from orderly translational motion of inner CNT to high frequency modes of outer CNT.

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