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Simulation of guitar string made with single-walled carbon nanotube

[1]Gbenro S. O., [2]Nchejane J. N., [3]Omole O. V.
[1]Department of Mathematical Science,
[1]Bamidele Olumilua University of Education, Science and Technology, Ikere-Ekiti, Nigeria
[2]Department of Mathematics and Computer Science,
[2]National University of Lesotho, Lesotho
[3]Department of Physics and Electronics,
[3]Bamidele Olumilua University of Education, Science and Technology, Ikere-Ekiti, Nigeria

Abstract: Using classical molecular dynamics (MD) and adaptive intermolecular reactive empirical bond order (AIREBO) potential, we perform simulations of guitar string made of single-walled carbon nanotube (SWCNT). The amplitude, the period and hence the frequency of oscillation of guitar string were determined. The effect of chirality on frequency of oscillation of nanotubes of fixed length was investigated for a guitar string rigidly clamped at different positions. The result shows that the frequency of oscillation is independent of the chirality of carbon nanotubes.

***IndexTerms* - single-walled carbon nanotube, simulation, guitar string, oscillation, zigzag, armchair.**

I. INTRODUCTION

Carbon nanotube was discovered by Sumio Iijima in 1991. Since then, the study of electronic, thermal and mechanical properties of single-walled carbon nanotubes (SWCNTs) has attracted a lot of attention and researches. Carbon nanotubes have great potential to collapse if the diameters of the tube go beyond stipulated threshold with great external force per unit area on their walls [1]. Carbon nanotubes (CNT) can be described as a tube that has translated the basic potentials in condensed matter physics over the years [2].

The characteristic of carbon nanotube arising from the unique combination of stiffness, low density and structural specificity has prompted many applications in the development of structurally specific materials at nanoscale [3]. The recent applications are found in field-emission displays, electrochemical energy storage, super capacitors, and nanoresistors while researches have advanced on possible usage in drug delivery systems, and biochemical sensors [4]. One of the foremost acoustic musical instruments used for musical styles for ages with a wide range of quality is the guitar. The acoustic guitars could transform sound generated from the string to energy with the aid of soundboards and the radiation from its flat components. Soundboards have a significant effect on the performance of guitars [5], [6], and [7].

Challenges arising from experimental procedures to understand the behavior of nanostructures under different loading conditions necessitate the adoption of molecular dynamics (MD) simulations. In this method, discrete solution of Newton's classical equations of motion is used to represent the dynamics of atoms or molecules of materials under investigation [8]. However, the challenge in this procedure is that the vibration modes of atoms dictate the time steps in the simulation [8].

[3] employed a classical MD simulation of SWCNTs constrained to an axial strain to study the axial strain induced torsion (a-SIT) response of SWCNT structure. The SWCNT characteristics considered were CNT curvature and chirality. They employed the reactive empirical bond order (REBO) potential to describe the carbon-carbon interactions. They concluded that a-SIT responses of SWCNT depend on both curvature and chirality.

[8] used MD simulation to investigate the impact of wave propagation, small scale parameter and chirality in SWCNTs using nonlocal Timoshenko beam theory. [9] used nanoelectromechanical procedure for electrical actuation and detection of guitar-string like oscillation modes of doubly clamped nanotube oscillators. It was shown that the vibration frequency can be greatly modified and that the system can be used to convert very small forces.

II. ATOMIC STRUCTURE OF THE SINGLE-WALLED CARBON NANOTUBES (SWCNTs)

Most single-walled nanotubes (SWNTs) have a diameter of about 1 nanometer with a tube length that can be many millions of times longer. The structure of a SWNT can be conceptualized by wrapping one atom-thick layer of graphite called graphene into a seamless cylinder. The way the graphene sheet is wrapped is represented by a pair of indices (n, m) called the chiral vector. The chiral vector is given by

$$\vec{C}_h = n\overrightarrow{a_1} + m\overrightarrow{a_2} = (n, m)$$

Where $\overrightarrow{a_1}$ and $\overrightarrow{a_2}$ are base vectors. The base vectors determine the chirality of the SWCNT and can appear in any of these three forms: zigzag, armchair, and chiral CNTs.

The chiral angle in terms of integer (n, m) is given by [10]

$$\theta = arccos\left(\frac{2n+m}{2\sqrt{m^2+n^2+mn}}\right)$$

The diameter of SWCNT in terms of integer (n, m) is given by [41]

$$d = a\sqrt{\frac{3(m^2+n^2+mn)}{n}}$$

Where a represents the carbon-carbon bond and has a value of $1.42\dot{A}$ [10].

III. SIMULATION OF GUITAR STRING

The simulation of guitar string is divided into two parts. The first simulation was done to determine the amplitude of the guitar string at which the elastic limit of the material is reached. The second set of simulations involved oscillation of the guitar string for different fractions of the maximum height.

3.1 First simulation

During the first simulation, the string is pulled in the middle with a velocity of 0.025nm/s in vertical direction while the two ends were fixed. We made a 1000 equilibration in 100K with temperature scaling. We obtained the amplitude of the strings at which the elastic limits are reached. See the figures below.

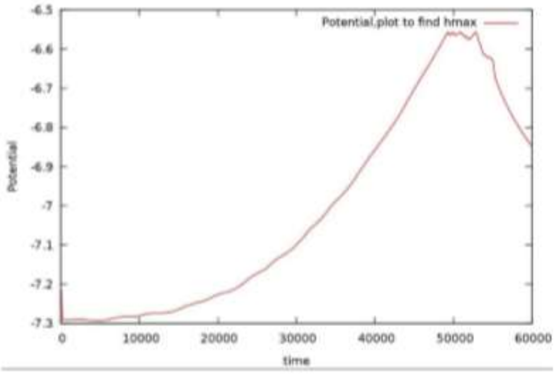


Figure 1: Time reach maximum height for guitar string made with Zigzag nanotube

From the plot in figure 1, the time to reach the maximum height for the guitar made with zigzag nanotube is t_{hmax}= 49.430s.

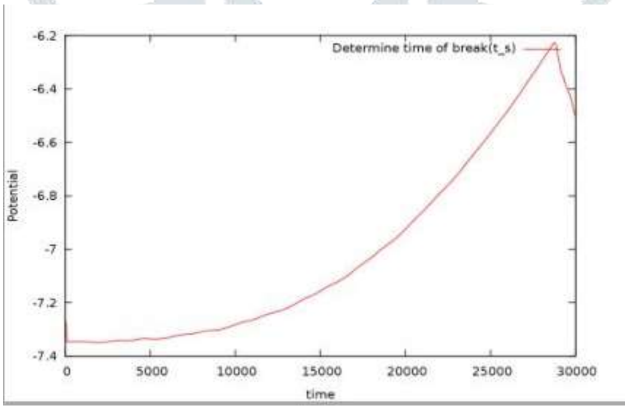


Figure 1: Time to reach maximum height for guitar string made with Armchair nanotube

From the plot in figure 1, the time to reach the maximum height for the guitar made with zigzag nanotube is t_{hmax} = 58,769s.

3.2 Second simulation

Simulations for $\frac{1}{3}t_{hmax}$, $\frac{2}{3}t_{hmax}$, and $\frac{9}{10}t_{hmax}$, were performed with temperature scaling switched off. Two cases were considered:

- First, the middle of the string was held up and the string could vibrate.
- Second, the whole string oscillates.

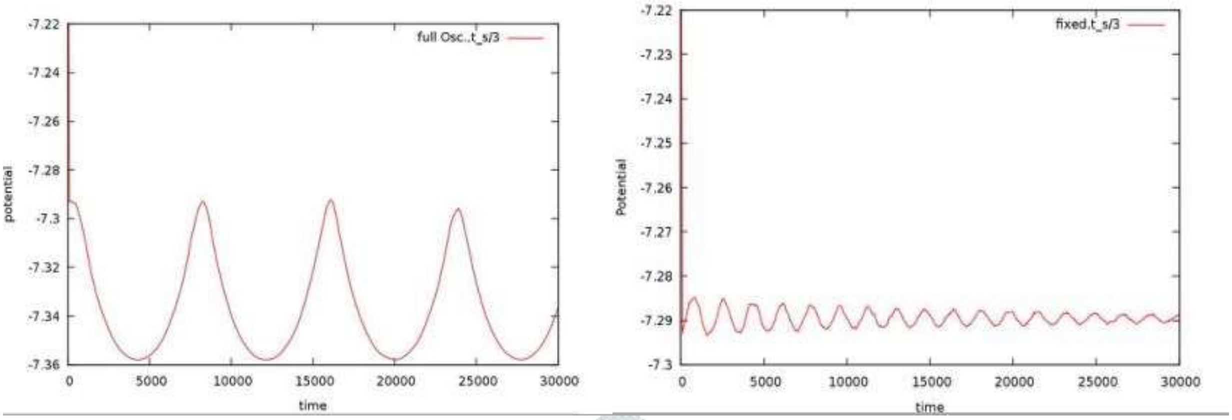
The results obtained enable us to determine the amplitude, the period and hence the frequency of the strings.

3.3 Determination of period and frequency of oscillation

In this section, we calculate the period and the frequency of oscillation of the both whole guitar string, and the case in which the middle is clamped.

3.3.1 String made with Zigzag nanotube

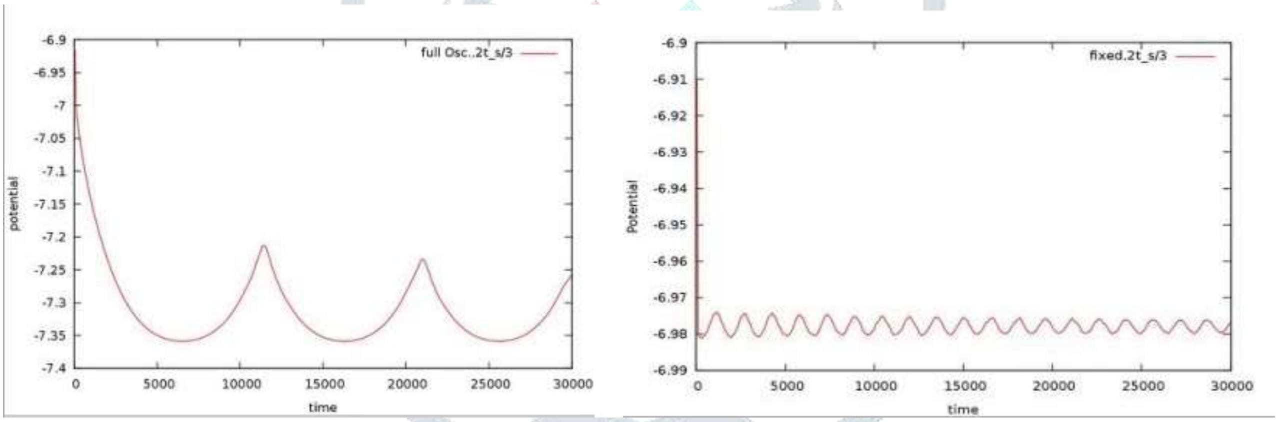
At $\frac{1}{3}t_{hmax}$:



(a) Oscillation of the whole guitar string (b) Oscillation of guitar string with fixed middle

For full Oscillation, the period $T = 1.459032 \times 10^{-11}s$, as determined from the plot in figure 3(a). The frequency is given by $f = \frac{1}{T}$. Thus, we have $f = 6.8539 \times 10^{10}hz$. With middle of the string fixed, $T = 4.08313 \times 10^{-12}s$, as determined from the plot in figure 3(b) Then $f = 2.4491 \times 10^{11}hz$.

At $\frac{2}{3}t_{hmax}$:

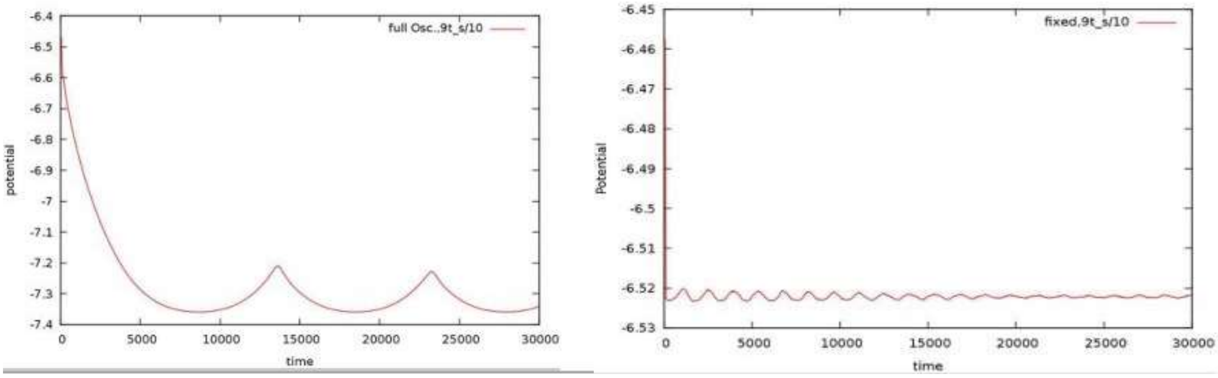


(a) Oscillation of the whole guitar string (b) Oscillation of guitar string with fixed middle

Figure 4: oscillation of Zigzag nanotube for $\frac{2}{3}t_{hmax}$

For full Oscillation, the period $T = 2.112332 \times 10^{-11}s$, as determined from the plot in figure 4(a). The frequency is $f = 4.7341 \times 10^{10}hz$. With the string fixed at the middle, we have $T = 3.04872 \times 10^{-12}s$, as determined from the plot in figure 4(b). Hence, the frequency is $f = 3.2801 \times 10^{11}hz$.

At $\frac{9}{10}t_{hmax}$:



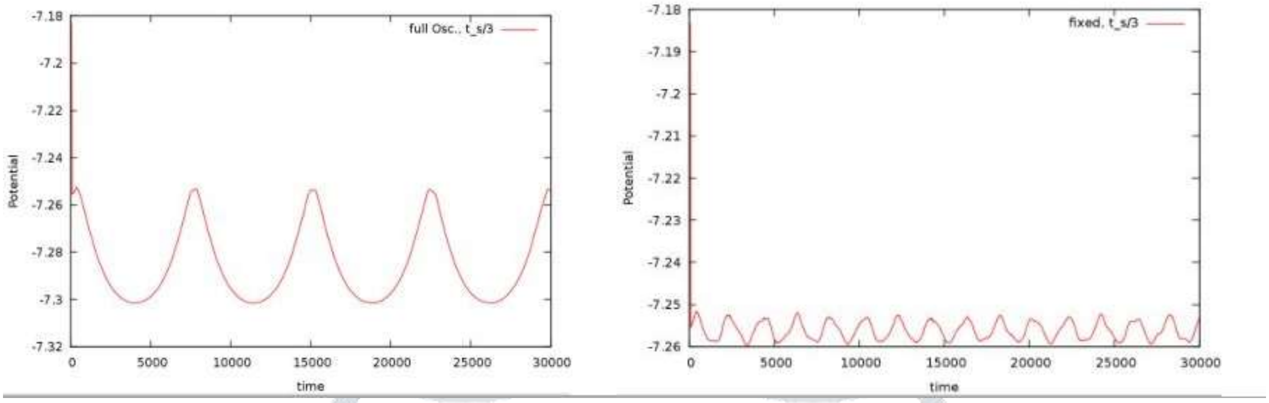
(a) Oscillation of the whole guitar string (b) Oscillation of guitar string with fixed middle

Figure 5: oscillation of Zigzag nanotube for $\frac{9}{10}t_{hmax}$

For full Oscillation, the period T = 1.61915 × 10−11s as determined from the plot in figure 5(a). The frequency is $f = 6.1761 \times 10^{10} hz$. With the string fixed at the middle, the period $T = 3.157607 \times 10^{-12} s$, as determined from the plot in figure 5(b). The frequency is $f = 3.1670 \times 10^{11} hz$.

3.3.2 String made with Armchair nanotube

At $\frac{1}{3}$t$_{\text{hmax}}$:

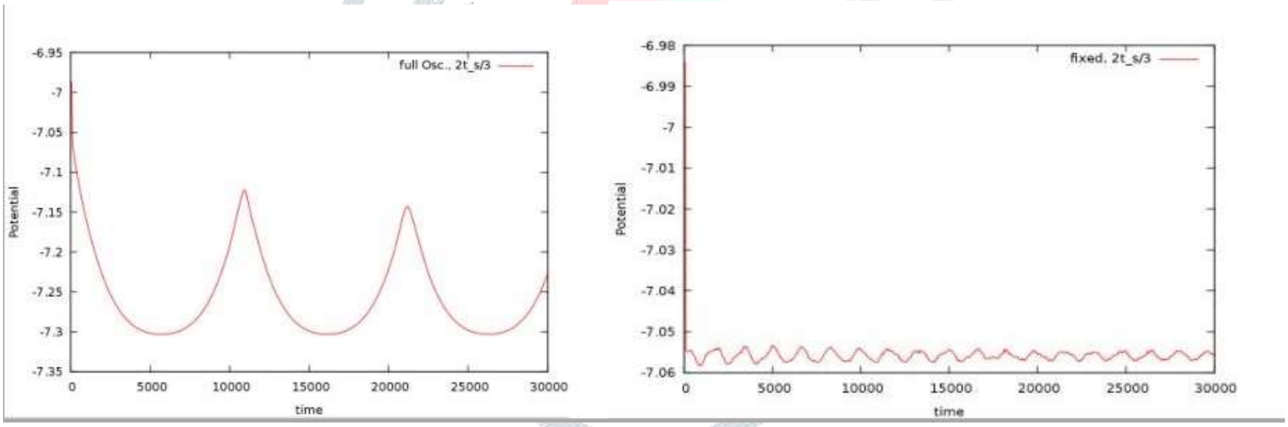


(a) Oscillation of the whole guitar string (b) Oscillation of guitar string with fixed middle

Figure 6: oscillation of Armchair nanotube for $\frac{1}{3}$t$_{\text{hmax}}$

For full Oscillation, the period $T = 1.567964 \times 10^{-11} s$, as determined from the plot in figure 6(a). The frequency is given by $f = \frac{1}{T}$. Thus, we have $f = 6.3777 \times 10^{10} hz$. With the middle of the string fixed, $T = 3.375374 \times 10^{-12} s$, as determined from the plot in figure 6(b). Then $f = 2.9626 \times 10^{11} hz$.

At $\frac{2}{3}$t$_{\text{hmax}}$:

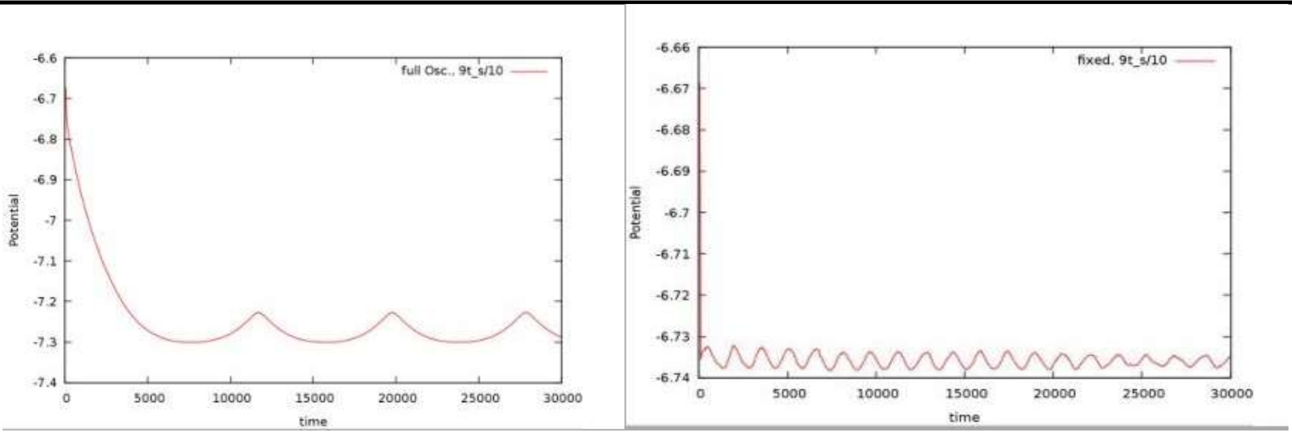


(a) Oscillation of the whole guitar string (b) Oscillation of guitar string with fixed middle

Figure 7: oscillation of Armchair nanotube for $\frac{2}{3}$t$_{\text{hmax}}$

For full Oscillation, the period $T = 1.932671 \times 10^{-11} s$, as determined from the plot in figure 7(a). The frequency is $f = 5.1742 \times 10^{10} hz$. With middle fixed, we have $T = 3.15759 \times 10^{-12} s$, as determined from the plot in figure 7(b). The frequency is $f = 3.1670 \times 10^{11} hz$

At $\frac{9}{10}$t$_{\text{hmax}}$:



(a) Oscillation of the whole guitar string (b) Oscillation of guitar string with fixed middle

Figure 8: oscillation of Armchair nanotube for $\frac{9}{10}t_{hmax}$

For full Oscillation, the period $T = 1.985515 \times 10^{-11} s$ as determined from the plot in figure 8(a). The corresponding frequency of oscillation is $f = 5.0364 \times 10^{10} hz$. With the string fixed in the middle, the period $T = 2.93984 \times 10^{-12} s$, as determined from the plot in figure 8(b). The corresponding frequency of oscillation is $f = 3.4015 \times 10^{11} hz$.

IV. **RESULT AND DISCUSSION**

Based on the formulation obtained above involving different chirality, vibration dynamics of single-walled carbon nanotubes (SWCNTs) are discussed here. The results, including the effect of chirality and the state of guitar string, are presented.

Based on molecular dynamics (MD) simulation with AIREBO potential, the vibration frequency for two types of single-walled carbon nanotubes (SWCNTs), zigzag and armchair CNTs, are calculated. It was observed that as time evolves, the period of oscillation for the armchair nanotube increases while that of zigzag nanotube which seems to be constant. The table below shows the type of nanotube, the state of string and the corresponding frequency measured in Giga Hertz (Ghz).

Table 1: Vibration frequency of guitar string made with SWCNT

Frequency of oscillation (Ghz)				
Nanotube	State of string	$\frac{1}{3}t_{hmax}$	$\frac{2}{3}t_{hmax}$	$\frac{9}{10}t_{hmax}$
Zigzag	Full oscillation	68.54	47.34	61.76
	Middle fixed	244.91	328.01	316.70
Armchair	Full oscillation	63.78	51.74	50.36
	Middle fixed	296.26	316.70	340.15

V. **CONCLUSION**

This paper studies the oscillatory properties of SWCNTs using molecular dynamics (MD) simulation with AIREBO potentials. The state of guitar string and the chirality of different nanotubes formed the basis of the investigation. The maximum period of oscillation was obtained for each type of SWCNTs and then the frequencies of oscillation were estimated through the MD simulation for different fractions of the maximum oscillatory period. The result indicated that the frequency of oscillation is independent of the chirality of the SWCNTs.

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