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Abstract

Carbon nanostructures, such as nanotubes and fullerenes, are of considerable interest to a wide range of research communities. Owing to their unique properties, a number of applications involving these structures have been proposed, one of which is the so-called nano-scaled oscillators, for which the resultant oscillatory frequencies are in the gigahertz range. The phenomena of the gigahertz oscillations have also led to the possible creation of future devices, such as ultra-fast optical filters and ultra-sensitive nano-antennae. In this paper we present recent developments in this area and review the authors recent work, where we investigate the mechanics of a new type of gigahertz oscillator comprising a fullerene C₆₀ oscillating within the centre of a uniform concentric ring or bundle of carbon nanotubes. Using the Lennard-Jones potential and the continuum approach, for which carbon atoms are assumed to be uniformly distributed across the surface of a molecule, we provide the underlying mechanisms of these nano-scaled oscillators.

Keywords

Mechanics, fullerene, carbon, nanotube, bundle, oscillators

Disciplines

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MECHANICS OF FULLERENE–CARBON NANOTUBE BUNDLE OSCILLATORS

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Key Words: Carbon nanotubes, Fullerenes, Carbon nanotube bundles, Gigahertz oscillators, Lennard-Jones potential

Abstract. *Carbon nanostructures, such as nanotubes and fullerenes, are of considerable interest to a wide range of research communities. Owing to their unique properties, a number of applications involving these structures have been proposed, one of which is the so-called nano-scaled oscillators, for which the resultant oscillatory frequencies are in the gigahertz range. The phenomena of the gigahertz oscillations have also led to the possible creation of future devices, such as ultra-fast optical filters and ultra-sensitive nano-antennae. In this paper we present recent developments in this area and review the authors' recent work, where we investigate the mechanics of a new type of gigahertz oscillator comprising a fullerene C_{60} oscillating within the centre of a uniform concentric ring or bundle of carbon nanotubes. Using the Lennard-Jones potential and the continuum approach, for which carbon atoms are assumed to be uniformly distributed across the surface of a molecule, we provide the underlying mechanisms of these nano-scaled oscillators.*

1 INTRODUCTION

Carbon nanotubes have received much attention for their possible application in many new nano-devices. Essentially, this is due to their unique properties, such as flexibility, high strength and low weight. Single-walled carbon nanotubes can be thought of as a graphene sheet rolled up to form a seamless cylinder. Their properties are strongly dependent on their bonding and geometric structure. The structure of a carbon nanotube is determined by the direction which the graphene sheet is rolled up. This direction can be identified by the so-called chiral vector \mathbf{C} , which is defined by $\mathbf{C} = n\mathbf{a}_1 + m\mathbf{a}_2$ or (n, m) , where n, m are integers and $\mathbf{a}_1, \mathbf{a}_2$ are the two basis vectors of the graphene sheet, as shown in Fig. 1. A carbon nanotube with $m = n$ is called armchair, $m = 0$ is a zigzag nanotube, and for arbitrary m and n it is termed chiral. Also, the radius of a (n, m) carbon nanotube can be determined from $r = |\mathbf{C}|/2\pi = |\mathbf{a}_1|(n^2 + nm + m^2)^{1/2}/(2\pi)$, noting that $|\mathbf{a}_1| = |\mathbf{a}_2|$.

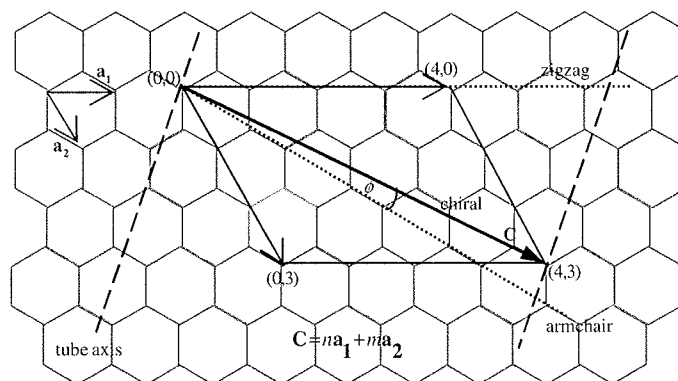


Figure 1: Chirality of carbon nanotubes.

Because carbon nanotubes display superior mechanical properties such as ultra high elastic moduli, strength and low mass density, they have potential applications in composite materials and other mechanical systems. Further, the deformations are elastic and completely reversible. The strong coupling between the electrical properties and mechanical deformation has many potential applications such as nano-scaled sensors and nano-electro-mechanical systems (NEMS). For details of the properties of carbon nanotubes, we refer the reader to Dresselhaus *et al.*¹, Harris², Rao *et al.*³ and Qian *et al.*⁴, for example. One other impact of carbon nanotubes to industrialized applications is their use to create nano-scaled oscillators for devices, such as ultra-fast optical filters and ultra-sensitive nano-antennae. In this paper, we review some of these developments and summarize the authors' recent work on mechanical and mathematical modelling for a new type of gigahertz nano-scaled oscillator, which is the C_{60} -nanotube bundle oscillator.

From experiments of Cumings and Zettl⁵ on pulling the inner core out and releasing it back into the outer shell of a multi-walled carbon nanotube, an ultra-low sliding frictional force is reported and it is also observed that the extruded core, after release, quickly and fully retracts

inside the outer shell due to the restoring force resulting from the van der Waals interaction acting on the extruded core. Based on these results, Zheng and Jiang⁶ and Zheng *et al.*⁷ use molecular dynamics simulations to study the sliding of the inner shell inside the outer shell of a multi-walled carbon nanotube, and they find that the oscillation can generate frequencies up to several gigahertz, and also that the frictional effect of the intershell sliding is very small, supporting the experimental findings of Cumings and Zettl⁵. This phenomenon is also confirmed by other molecular dynamics studies, such as Legoas *et al.*⁸ and Rivera *et al.*^{9,10}. Further, to model the force distribution for double-walled carbon nanotubes and the oscillation of the inner tube inside the outer tube, Boawan and Hill¹¹ use the continuum approach for the Lennard-Jones potential and Newton's second law, where the frictional force is neglected. They obtain an exact analytical expression for the interaction energy between the inner and outer tubes and the van der Waals interaction force. This model also predicts gigahertz oscillatory frequencies as expected for the double-walled carbon nanotube oscillator.

From Zheng *et al.*⁷ it is observed that the shorter the inner tube, the higher the frequency, and this leads to the molecular dynamics study of Liu *et al.*¹² who find that a higher frequency can be generated by the oscillation of a C₆₀ fullerene inside a single-walled carbon nanotube. We note that a C₆₀ fullerene, also known as a buckyball, is one of many forms of stable carbon structures, where sixty carbon atoms bond to form a single approximately spherical cage-like molecule. We refer the reader to Dresselhaus *et al.*¹ for further details of fullerenes. We find that the study of the interaction between a C₆₀ fullerene and a single-walled carbon nanotube has previously been studied by Qian *et al.*¹³. While Liu *et al.*¹² focus on the oscillation frequency, the study of Qian *et al.*¹³ is concerned with the suction (or repulsion) of a C₆₀ fullerene at the vicinity of the carbon nanotube open end and the velocity of the fullerene upon entering the nanotube. The molecular dynamics simulations of Qian *et al.*¹³ motivate Cox *et al.*^{14,15} to study this problem from an applied mathematical modelling perspective. In particular, Cox *et al.*¹⁴ employ elementary mechanical principles, utilizing the continuum approach to provide a classical applied mathematical model, which enables the determination of an analytical expression for the suction energy of a C₆₀ molecule upon entering a carbon nanotube. This energy is imparted onto the C₆₀ molecule in terms of kinetic energy and thus induces the oscillating motion. Cox *et al.*¹⁴ also determine the condition on the radius of carbon nanotubes that will accept the C₆₀ molecule at rest in the vicinity of an open end of the tube. In Cox *et al.*¹⁵, a novel mathematical model for the oscillation of the C₆₀-carbon nanotube oscillators is provided where the axial van der Waals restoring force of the C₆₀ molecule is approximated by two equal and opposite Dirac delta functions operating at both ends of the nanotube. We note that the results of the classical mathematical model of Cox *et al.*^{14,15} are shown to be in good agreement with numerical results of Girifalco *et al.*¹⁶ and Hodak and Girifalco¹⁷, and molecular dynamics simulations of Liu *et al.*¹² and Qian *et al.*¹³.

Recently, a new type of nano-scaled oscillator has been reported, which are known as carbon nanotube bundle oscillators. Using molecular dynamics simulations, Kang *et al.*¹⁸ propose the new oscillator based on a single-walled carbon nanotube oscillating within a bundle of six similar carbon nanotubes. By adopting similar techniques to those in Cox *et al.*^{14,15}, the same

authors¹⁹ investigate carbon nanotube bundle oscillators, for which the inner oscillating molecules is a single-walled carbon nanotube. Since much higher frequencies can be generated from a C₆₀ fullerene oscillating inside a nanotube, Cox *et al.*²⁰ extend their analysis of nanotube-bundle oscillators to also consider the special case of a C₆₀ fullerene oscillating within a bundle of carbon nanotubes. We note that a more general definition of a bundle than that of Kang *et al.*¹⁸ is adopted in Cox *et al.*^{19,20}, which is a bundle that is assumed to comprise an integral number of N carbon nanotubes aligned parallel to and equidistant from a common axis, which is termed the bundle axis. The perpendicular distance from the bundle axis to the axis of each constituent nanotube is termed the bundle radius R . It is also assumed that the constituent nanotubes are all of equal length $2L$ and radius r and they are evenly distributed around the bundle axis, so that the angle subtended at the bundle axis of two adjacent nanotubes is $2\pi/N$. Noting that when $N = 6$, the results for nanotube-bundle oscillators are consistent with those shown of Kang *et al.*¹⁸.

2 INTERACTION ENERGY

For the interaction energy between two atoms, we adopt the Lennard-Jones potential which is given by $\Phi = -Ar^{-6} + Br^{-12}$, where r denotes the distance between two interacting atoms and A and B are attractive and repulsive constants, respectively. For the interaction between two carbon nanostructures, we adopt the continuum approach for which the atoms are assumed to be uniformly distributed over the surface of a molecule, thus the total interaction energy is given by

$$E = \eta_1 \eta_2 \int \int_{S_1 S_2} \Phi(\rho) dS_1 dS_2, \quad (1)$$

where here η_1 and η_2 denote the mean atomic densities of atoms on each molecule and ρ is the distance between two typical surface elements dS_1 and dS_2 on each molecule.

In order to obtain the interaction energy of a carbon nanotube bundle, we first assume that the geometry of the bundle is described as in the Introduction, so that we can prescribe a surface of the i th nanotube in the bundle in terms of the Cartesian coordinates (x, y, z) by

$$\left(R \cos\left(\frac{2\pi(i-1)}{N}\right) + r \cos\theta_i, R \sin\left(\frac{2\pi(i-1)}{N}\right) + r \sin\theta_i, z_i \right),$$

where $i \in \{1, \dots, N\}$, $0 \leq \theta_i \leq 2\pi$ and $-L \leq z_i \leq L$. We note that in parts of section 3 it is convenient to assume $0 \leq z_i \leq \infty$ or assume $-\infty \leq z_i \leq \infty$. For the interaction between two parallel carbon nanotubes, Cox *et al.*¹⁹ adopt (1) to derive the analytical expression for the potential energy per unit length, E_u , in terms of the Appell hypergeometric functions of two variables as

$$E_u = \frac{3}{2} \eta_1^2 r_1 r_2 \pi^3 \alpha^{-5} \left[-A F_2 \left(\frac{5}{2}, -\frac{3}{2}, \frac{1}{2}, 1, 1; -\frac{r_1^2}{\alpha^2}, -\frac{4r_2 \delta}{\alpha^2} \right) + \frac{21}{32} B \alpha^{-6} F_2 \left(\frac{11}{2}, -\frac{9}{2}, \frac{1}{2}, 1, 1; -\frac{r_1^2}{\alpha^2}, -\frac{4r_2 \delta}{\alpha^2} \right) \right], \quad (2)$$

where η_t is the mean atomic density of a carbon nanotube, δ denotes the distance between the axes, r_1 and r_2 are radii of the tubes, $\alpha^2 = (\delta - r_2)^2 - r_1^2$ and $F_2(a, b, b', c, c'; x, y)$ is an Appell hypergeometric function of two variables of the second kind as defined by Erdelyi *et al.*²¹. Thus, using (2) we can determine the total interaction energy E_B of a bundle comprising N nanotubes each of which has radius r by summing over all of the constituent interactions, namely

$$E_B = \frac{N}{2} \sum_{k=1}^{N-1} E_{tt} \left(2R \sin \left(\frac{k\pi}{N} \right) \right). \quad (3)$$

As the interactions between nanotubes in a bundle are dominated by the nearest neighbour interactions, we can approximate the total energy of the bundle to be given by

$$E_B \approx NE_{tt} (2R \sin(\pi/N)). \quad (4)$$

If we assume that nanotubes in a bundle arrange themselves such that the bundle configuration is at equilibrium (i.e. the energy is minimum), then we can determine the bundle radius R from (4). In Fig. 2, we show the relation between the bundle radius R and the tube radius r which minimizes the energy E_B of the system. If we let λ be the equilibrium interspacing between two tubes when the interaction energy is minimized, then as shown in Cox *et al.*¹⁹, we can predict that the bundle radius R is given by $R \approx (2r + \lambda)/[2\sin(\pi/N)]$. We also find that λ varies slightly as a function of the nanotube radius, but generally lies in the range 3.10–3.16 Å.

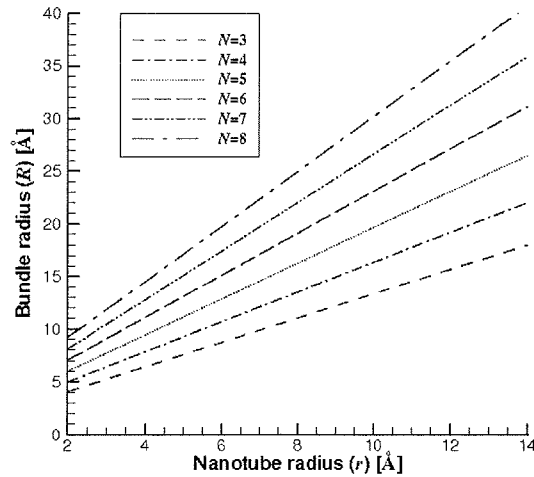


Figure 2: Bundle radius versus nanotube radius for bundles with $N \in \{3, 4, \dots, 8\}$ at minimum energy configuration²⁰.

3 INTERACTION BETWEEN A C₆₀ FULLERENE AND NANOTUBE BUNDLES

The study of a fullerene oscillating inside a single-walled carbon nanotube^{14,15} and the study of a carbon nanotube oscillating in a bundle¹⁹ leads to the examination of other possible types

of a gigahertz oscillator, which are created from a fullerene oscillating in the centre of a nanotube bundle. In this section, we summarize the results of Cox *et al.*²⁰ for this novel nano-scaled oscillator.

3.1 Interaction of fullerenes with bundles

As shown in Cox *et al.*²⁰, the total interaction energy of a fullerene radius of r_0 located at the centre of a nanotube bundle of infinite in length is given by

$$W = -\sum_{k=1}^N E_{f_i}(R), \quad (5)$$

where R the bundle radius, is the distance from the centre of the fullerene to the axis of the nanotubes in the bundle and E_{f_i} denotes the interaction energy between the fullerene and a single nanotube which is derived in Cox *et al.*¹⁴, namely

$$E_{f_i}(R) = 4\pi^2 r_0^2 r \eta_f \eta_t \left[\frac{B}{5} \left(\frac{315}{256} J_5 + \frac{1155}{64} r_0^2 J_6 + \frac{9009}{128} r_0^4 J_7 + \frac{6435}{64} r_0^6 J_8 + \frac{12155}{256} r_0^8 J_9 \right) - \frac{A}{8} (3J_2 + 5r_0^2 J_3) \right],$$

where η_f is the mean atomic density of the fullerene and J_n is defined in terms of the usual hypergeometric function as

$$J_n = \frac{2\pi}{\left[(r-R)^2 - r_0^2 \right]^{n+1/2}} F \left(\frac{1}{2}, n + \frac{1}{2}; 1; -\frac{4rR}{(r-R)^2 - r_0^2} \right).$$

From (5), we can find the bundle radius which optimizes the suction energy for a particular tube radius r . In the other words, for any value of N we can determine the relationship between the nanotube radius r and the bundle radius R which optimizes the suction energy for the C_{60} fullerene, and this is shown graphically in Fig 3. On the same figure, we also show the nanotube radii versus bundle radii data from Fig. 2. The points where the lines intersect represent the specific values of r and R that lead to optimized oscillators which operate at the highest frequency for specific values of N . From Fig. 3, it can be seen that if we limit the tube radius r to 2-12 Å then the C_{60} -bundle oscillators can only be constructed for $N \in \{4, 5, 6, 7\}$. In Table 1, we present the parameters of the oscillators which optimize the suction energy. As the suction energy is directly converted into kinetic energy, results shown in Table 1 are particularly important as guidelines for constructing bundle oscillators that achieve the maximum velocity and frequency.

Number N	Tube radius r (Å)	Bundle Radius R (Å)	Suction energy W_f (eV)
4	10.294	16.792	2.314
5	5.439	11.930	2.551
6	3.355	9.838	2.731
7	2.219	8.692	2.850

Table 1: parameters for optimized C_{60} -bundle oscillators²⁰.

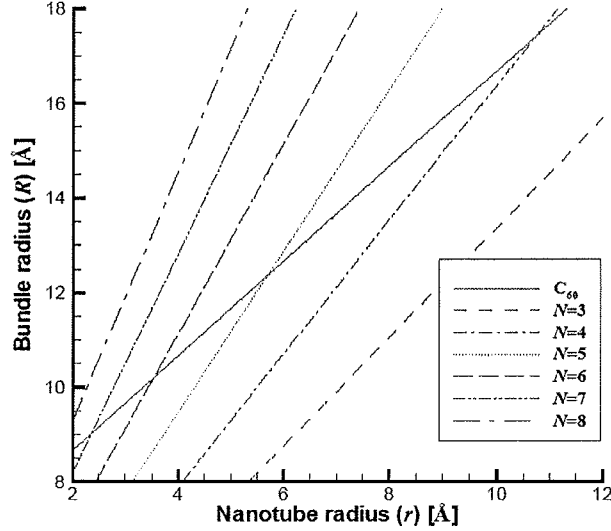


Figure 3: Bundle radius versus nanotube radius for a C_{60} fullerene nanotube bundles with $N \in \{3, 4, \dots, 8\}$ ²⁰.

3.2 Suction of fullerenes into bundles

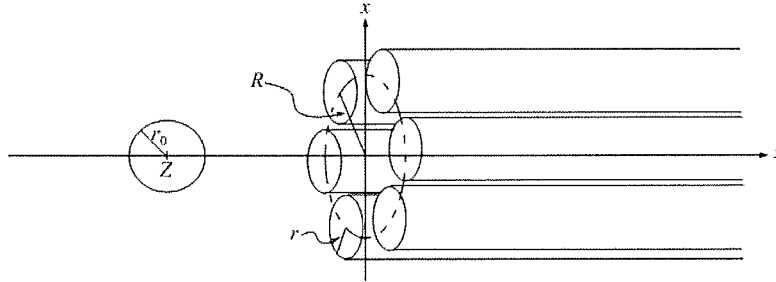
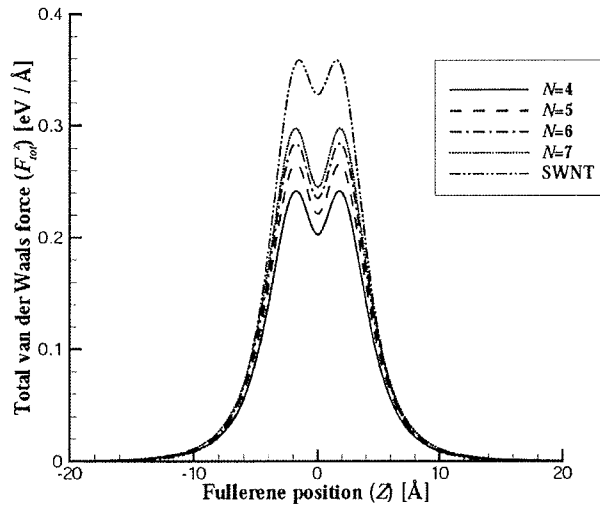
For a C_{60} fullerene centered at $(0, 0, Z)$ and radius r_0 interacting with a bundle comprising semi-infinite carbon nanotubes, as shown in Fig. 4, the total van der Waals interaction force can be obtained from $F_{tot}^z = NF_{vdw}^z$, where F_{vdw}^z is the van der Waals force for a fullerene interacting with a single nanotube. As shown in Cox *et al.*²⁰, F_{vdw}^z is evaluated analytically and is given by

$$F_{vdw}^z(Z) = 4\pi r r_0^2 \eta_t \eta_f \left[A(I_3 + 2r_0^2 I_4) - (B/5)(5I_6 + 80r_0^2 I_7 + 336r_0^4 I_8 + 512r_0^6 I_9 + 256r_0^8 I_{10}) \right],$$

where I_n can be given in the form

$$I_n = 2\pi(\mu + 4rR)^{1/2-n} \sum_{m=0}^{n-1} \frac{(1-n)_m (1/2)_m}{(m!)^2} (-4rR)^m \mu^{-1/2-m},$$

where $\mu = (R-r)^2 - r_0^2 + Z^2$ and $(\alpha)_m$ denotes the Pochhammer symbol $(\alpha)_m = \alpha(\alpha+1)(\alpha+2)\dots(\alpha+m-1)$. In Fig. 5, we show the force profiles for the four optimal oscillator configurations presented in Table 1, together with that of a C_{60} -single walled nanotube interaction from Cox *et al.*¹⁴ with the nanotube radius 6.783 Å. From the figure, the force is positive implying that the C_{60} fullerene is sucked into the bundle. It also can be seen from Fig. 5 that the force for bundle oscillators is significantly less than that generated by the optimal C_{60} -nanotube oscillator. As described in Cox *et al.*²⁰, the higher force from the C_{60} -nanotube oscillator is due to the fact that the curvature of the nanotube wall matches the curvature of the oscillating fullerenes and therefore a greater van der Waals force can be operated in the optimum distance.

Figure 4: Geometry for a C_{60} fullerene entering a nanotube bundle.Figure 5: Total van der Waals force for a fullerene entering a nanotube bundle for various configurations²⁰.

3.3 Oscillating of fullerenes inside bundles

Since the force profiles for C_{60} -bundle oscillators are similar to those of C_{60} -single-walled carbon nanotube oscillators¹⁵, the model presented in Cox *et al.*¹⁵, which involves approximating the forces operating at both ends of the bundle as Dirac delta functions, can also be used for C_{60} -bundle oscillators. Using the equation for frequency $f = (2W_f / m_f)^{1/2} / (4L)$ where m_f is the mass of the fullerene, we plot Fig. 6 showing the oscillatory frequencies for various bundle oscillators, varying the bundle length $2L$. As expected from Table I, the configuration with $N = 7$ gives rise to the highest frequency. As also expected, the frequency obtained from a C_{60} oscillating in a single-walled nanotube is higher than that of the C_{60} -bundle oscillators presented here.

4 SUMMARY

In summary, this paper reviews some developments involving nano-scaled gigahertz oscillators and provides a synopsis of recent work of the authors on modelling the

mechanisms of a new type of nano-oscillators, which is the C_{60} -bundle oscillator. By using the Lennard-Jones potential together with the continuum approach, the formal mathematical expressions of the energy and the van der Waals interaction force are determined. The results obtained can be used to predict the oscillator bundle configuration which optimizes the suction energy and therefore leads to a maximum frequency oscillator. We emphasize that the major contribution of the authors in this area is the use of elementary mechanics and classical applied mathematics to formulate explicit analytical solutions and ideal model behaviour in a scientific context previously only elucidated through experiments and molecular dynamics studies.

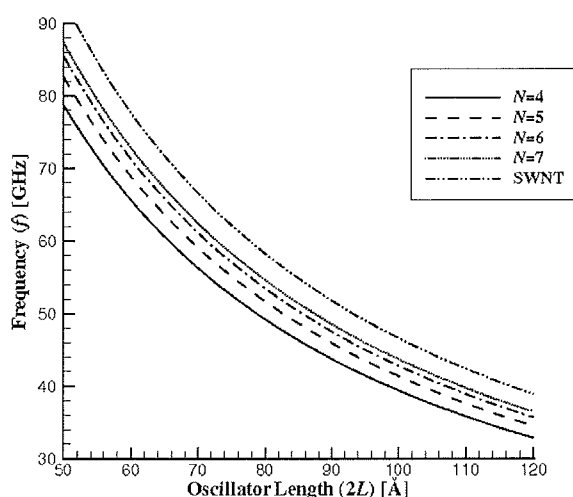


Figure 6: Frequency for a fullerene nanotube bundle oscillator for various configurations and for a fullerene oscillating in a single-walled carbon nanotube²⁰.

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