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Torsional vibration of carbon nanotube–buckyball systems based on nonlocal elasticity theory

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ABSTRACT

In this paper, torsional vibration analysis of single-walled carbon nanotube–buckyball systems is carried out. The buckyball is attached to single-walled carbon nanotube (SWCNT) at one end and the other end of SWCNT is fixed. Such nanostructures are promising for tunable nanoresonators whose frequency can be altered by attaching different buckyballs. Nonlocal elasticity is utilized to examine the small-scale effect on the nanoresonators and derive the torsional frequency equation and nonlocal transcendental equation. Based on these equations, numerical results are obtained for the dependence of the frequency on the mass moment of inertia. The analytical expressions of nonlocal frequencies are also derived when the buckyballs mass moment of inertias are much larger than that of SWCNTs. In addition, effort is made to study the influence of nonlocal parameter and attached buckyball on the torsional frequency of the nanoresonators.

1. Introduction

The invention of carbon nanotubes (CNTs) by Iijima [1] has opened a new world of research in the field of nanosensors, nanoresonators, nanodevices, nanoelectronics and nanocomposites. Various other new fields of utilization of CNTs are everyday explored. These nano-size structures exhibit superior physical, mechanical, chemical, electronic and electrical properties [2–5]. As cylindrical fullerenes are known as CNTs, spherical fullerenes are referred to as buckyballs [6–7]. Buckyballs are cage-like fused-ring polycyclic system of generally carbon atoms. As nanobuds [8] can be obtained by adjoining fullerene to CNT span, buckyballs can be incorporated at the tip of CNTs. The nanobuds are new structures where spherical fullerenes are covalently bonded to the outer sidewalls of the underlying nanotube. By similar method buckyballs can be fixed to the ends of nanotubes. When buckyballs are added to the both ends of nanotube we get a nano-dumbbell. These CNT–buckyball systems can be utilized as state-of-art filler materials for strong tough nanocomposites. Further the system can be used as tunable nanoresonator. The resonant frequency is sensitive to the resonator mass. The change in the attached mass on the resonator causes a shift to the resonant frequency. Attached buckyballs or added atoms at the tip of a SWCNT can influence frequency change in vibrating systems [9]. CNTs with added buckyballs can be effectively used as tunable resonators in nano-electro-mechanical-systems (NEMS) application.

Experiments at the nanoscale are extremely difficult and atomistic modeling remains prohibitively expensive for large-sized atomic system. Consequently size-dependent continuum models continue to play an essential role in the study of carbon nanotubes. The main reason these size-dependent continuum mechanics are used is because at small length scales the material microstructures (such as lattice spacing between individual atoms) become increasingly significant and its influence can no longer be ignored. Literature showed that nonlocal elasticity approach [10–26] is a popular method for modeling mechanical behavior of nanostructures, viz. nanotubes and graphenes. In nonlocal elasticity theory the small-scale effects are captured by assuming that the stress at a point as a function not only of the strain at that point but also of the strains at all other points of the domain [27]. This is in accordance with predictions from atomic lattice dynamics.

Using nonlocal elasticity theory, works on vibration, bending and buckling of carbon nanotubes are numerous. Most of the works are based on only explicit carbon nanotubes with no added mass. Nanotubes with added mass can be made as nanoresonators. Using classical mechanics theory and molecular mechanics, Adhikari and Chowdhury [9] has studied the bending vibration characteristics of carbon nanotubes with added mass. However limited numbers of works are found in literature that addresses nonlocal frequency analysis of CNTs with added mass. Lee et al. [28] has used nonlocal elasticity theory for study of the frequency shift and sensitivity of carbon nanotube-based sensor

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with an attached mass. Recently Murmu and Adhikari [29] have reported the longitudinal vibration of CNTs with attached buckyballs based on nonlocal elasticity theory.

In view of the above discussions, in this paper, we study the torsional vibration of single-walled-carbon-nanotubes (SWCNTs) with attached buckyballs. For the abovementioned problems we derive the governing equations for torsional vibration of coupled system based on nonlocal elasticity theory [10–29]. Analytical expressions of nonlocal torsional frequencies are derived when the mass of the attached buckyball is larger than the mass of SWCNT. Closed-form nonlocal transcendental equation for vibrating system with arbitrary mass (moment of inertia) ratio, i.e. mass of buckyball to mass of SWCNT, is derived. The frequency shifts due to (i) added buckyballs and (ii) nonlocal effects or small-scale effects are considered for arbitrary mass (moment of inertia) ratios. In summary, the following results and discussion of this study can be helpful for the design of a tunable nanoresonator.

2. Nonlocal elasticity approach

For the sake of completeness in this paper, we provide a brief review of the theory of nonlocal elasticity [27]. According to nonlocal elasticity, the basic equations for an isotropic linear homogenous nonlocal elastic body neglecting the body force are given as

$$\begin{aligned}
&\sigma_{ij,j}=0\\
&\sigma_{ij}(\mathbf{x})=\int_{\mathbf{V}}\phi(|\mathbf{x}-\mathbf{x}'|,\alpha)t_{ij}d\mathbf{V}(\mathbf{x}'),\ \forall\mathbf{x}\in\mathbf{V}\\
&t_{ij}=H_{ijkl}\varepsilon_{kl}\\
&\varepsilon_{ij}=\tfrac{1}{2}(u_{i,j}+u_{j,i})
\end{aligned}\tag{1}$$

The terms σ_{ij}, t_{ij} ε_{kl} and H_{ijkl} are the nonlocal stress, classical stress, classical strain and fourth order elasticity tensors, respectively. The volume integral is over the region $\mathbf{V}$ occupied by the body. The above equation (Eq. (1)) couples the stress due to nonlocal elasticity and the stress due to classical elasticity. The kernel function $\phi(|\mathbf{x}-\mathbf{x}'|,\alpha)$ is the nonlocal modulus. The nonlocal modulus acts as an attenuation function incorporating into constitutive equations the nonlocal effects at the reference point $\mathbf{x}$ produced by local strain at the source $\mathbf{x}'$. The term $|\mathbf{x}-\mathbf{x}'|$ represents the distance in the Euclidean form and α is a material constant that depends on the internal (e.g. lattice parameter, granular size and distance between the C–C bonds) and external characteristics lengths (e.g. crack length and wave length). Material constant α is defined as $\alpha=e_0a/\ell$. Here e_0 is a constant for calibrating the model with experimental results and other validated models. The parameter e_0 is estimated such that the relations of the nonlocal elasticity model could provide satisfactory approximation to the atomic dispersion curves of the plane waves with those obtained from the atomistic lattice dynamics. The terms a and ℓ are the internal (e.g. lattice parameter, granular size and distance between C–C bonds) and external characteristic lengths (e.g. crack length and wave length) of the nanostructure.

Eq. (1) is in partial-integral form and generally difficult to solve analytically. Thus a differential form of nonlocal elasticity equation is often used. According to Eringen [27], the expression of nonlocal modulus can be given as

$$\phi(|\mathbf{x}|,\alpha)=(2\pi\ell^2\alpha^2)^{-1}K_0(\sqrt{\mathbf{x}\cdot\mathbf{x}}/\ell\alpha)\tag{2}$$

where K_0 is the modified Bessel function.

Using Eqs. (1) and (2), the nonlocal constitutive can be approximated as

$$(1-\alpha^2\ell^2\nabla^2)\sigma_{ij}=t_{ij}\tag{3}$$

where ∇^2 is the Laplacian. Next we develop the equations for torsional vibration of carbon nanotubes.

3. Nonlocal torsional vibration of nanotube–buckyball system

Consider a single-walled carbon nanotube (SWCNT) with attached buckyball (Fig. 1a) undergoing torsional vibration. The SWCNT is assumed to be of length L. The mathematical idealization of the vibrating system is shown in Fig. 1b. General physical model to represent SWCNT include the nonlocal shell, nonlocal beam or nonlocal rod model. Here we will consider a simple one-dimensional nonlocal model. The present work can be extended to nonlocal shell model. In the present study, the SWCNT is considered to be slender and modeled by nonlocal rod theory. The nonlocal constitutive relation for shear stress in one-dimensional differential form can be simplified as [14]

$$\tau-(e_0a)^2\frac{\partial^2\tau}{\partial x^2}=G\gamma\tag{4}$$

where G is the shear modulus and γ is the shear strain. Term τ denotes the shear stress of SWCNT.

The stress resultant due to shear stress is written as

$$S=\int_A\tau\,dA\tag{5}$$

where A is the cross-section of the uniform SWCNT,

and the torque relation is given as

$$T=\int_A\tau z\,dA\tag{6}$$

By using Eqs. (4)–(6), we get the constitutive relation as

$$S-(e_0a)^2\frac{\partial^2S}{\partial x^2}=GA\gamma\tag{7}$$

$$T-(e_0a)^2\frac{\partial^2T}{\partial x^2}=GI_P\frac{\partial\theta}{\partial x}\tag{8}$$

where θ and I_P are the angular displacement and the polar moment of inertia of the cross-section of the SWCNT, respectively.

Considering an element of the SWCNT, equation of motion can be written as

$$\left(T+\frac{\partial T}{\partial x}dx\right)-T+T_{ext}\,dx=\rho I_P\frac{\partial^2\theta}{\partial t^2}dx\tag{9}$$

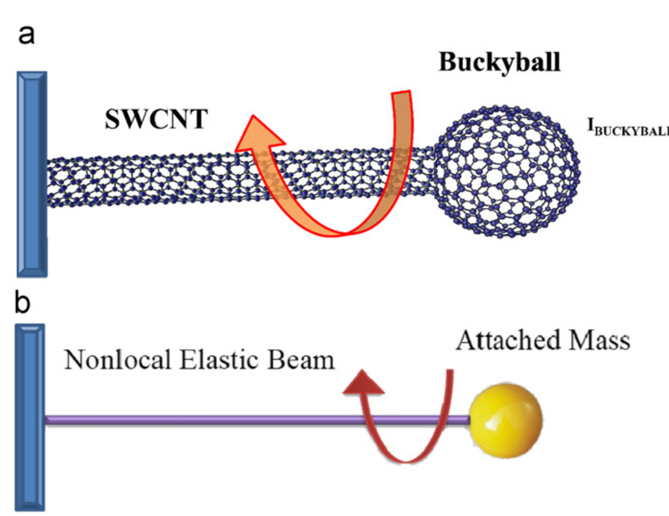

Fig. 1. (a) Torsional vibration of carbon nanotubes with attached buckyballs at tip, (b) mathematical idealization of nonlocal beam with attached mass.

where T and T_{ext} are the induced torque and the external torque per unit length, respectively. The term $\rho I_P \partial^2\theta/\partial t^2\, dx$ on the right hand side of Eq. (9) represents the inertia torque acting on the element of SWCNT. Terms ρ and t are the density of SWCNT and time, respectively.

Using Eqs. (8) and (9), we have

$$T = GI_P\frac{\partial\theta}{\partial x} + (e_0a)^2\left(\rho I_P\frac{\partial^2\theta}{\partial x\partial t^2} - \frac{\partial T_{ext}}{\partial x}\right) \tag{10}$$

Making use of equilibrium equation (Eq. (9)) and ignoring external torque we get the governing equation as

$$GI_P\frac{\partial^2\theta}{\partial x^2} = \rho I_P\frac{\partial^2\theta}{\partial t^2} - (e_0a)^2\rho I_P\frac{\partial^4\theta}{\partial x^2\partial t^2} \tag{11}$$

or using shear speed of sound $c=\sqrt{G/\rho}$, we have

$$\frac{\partial^2\theta}{\partial x^2} = (1/c^2)\frac{\partial^2\theta}{\partial t^2} - (e_0a)^2(1/c^2)\frac{\partial^4\theta}{\partial x^2\partial t^2} \tag{12}$$

when we neglect the nonlocal or small-scale effect (i.e. $e_0a=0$), we get the conventional scale-free equation for torsional vibration.

We assume the solution of Eq. (12) as

$$\theta(x,t) = \psi(x)e^{i\omega t} \tag{13}$$

where ω is the natural frequency and $i=\sqrt{-1}$. Considering normalizing coordinate, $X=x/L$ and using Eq. (9) (and neglecting T_{ext}) can be transformed to space variables form as

$$\frac{d^2\psi(X)}{dX^2} + \lambda^2\psi(X) = 0 \tag{14}$$

where

$$\lambda^2 = \frac{\Omega^2}{[1-(e_0a/L)^2\Omega^2]} \tag{15}$$

and

$$\Omega^2 = \omega^2L^2/c^2 \tag{16}$$

Solution of differential Eq. given in Eq. (14) can be expressed as

$$\psi(X) = A\cos\lambda X + B\sin\lambda X \tag{17}$$

where A and B are determined from boundary conditions.

In what follows we consider SWCNTs with one end fixed (at $X=0$) and a buckyball attached to the other end (at $X=1$) (Fig. 1). When the attached buckyball undergoes torsion the boundary conditions for such SWCNTs are as follows:

$$(\theta)_{X=0} = 0 \tag{18}$$

and

$$\left(\frac{GI_P}{L}\right)\left(\frac{\partial\theta}{\partial X}\right)_{X=1} + (e_0a)^2\left(\frac{\rho I_P}{L}\right)\left(\frac{\partial^3\theta}{\partial X\partial t^2}\right)_{X=1} = -I_{Buckyball}\left(\frac{\partial^2\theta}{\partial t^2}\right)_{X=1} \tag{19}$$

Here $I_{Buckyball}$ denotes the mass moment of inertia of the carbon buckyball. It should be noted that boundary condition represented by Eq. (19) is the nonlocal boundary condition. Eq. (19) is deduced from the torque balance relations in SWCNT–buckyball system at the tip where the buckyball is fixed. When e_0a becomes zero, i.e., nonlocal effect is neglected, it reduces to the classical one.

Substituting Eqs. (13) and (17) into boundary conditions (18) and (19) leads to the following governing nonlocal transcendental frequency equation:

$$1/\Delta I = \lambda\tan\lambda \tag{20}$$

where the term λ is defined by Eq. (15) and ΔI is the ratio of mass polar moment of inertia of the buckyball to the mass inertia of the SWCNT, i.e.

$$\Delta I = \frac{I_{Buckyball}}{I_{CNT}} \tag{21}$$

Here I_{CNT} is equal to $\rho I_P L$.

Considering $M_{Buckyball}$ as the mass of the buckyballs, and $R_{Buckyball}$ as the radius of the buckyballs, we obtain moment of inertia expression by standard spherical relation [30].

The mass moment of inertias of the buckyball is given by

$$I_{Buckyball} = (2/3)M_{Buckyball}R^2{}_{Buckyball} \tag{22}$$

Assuming the volume of buckyball as $(4/3)\pi R^3_{Buckyball}$ we consider the approximate effective radii of buckyball as

$$R_{Buckyball} = \sqrt[3]{\frac{0.2387M_{Buckyball}}{\rho_{Buckyball}}} \tag{23}$$

Similarly, considering M_{CNT} as the mass of the CNT, and R_{CNT} as the radius of the CNT we find mass moment of inertia by standard cylindrical relation [30]. The moment of inertias of the CNTs can be thus be assumed as

$$I_{CNT} = (1/2)M_{CNT}R^2{}_{CNT} \tag{24}$$

When the SWCNT is without attached buckyball, we have $\Delta I=0$. Thus eigenvalue equation ($\cos\lambda = \Delta I\lambda\sin\lambda$) reduces to conventional frequency equation:

$$\cos\lambda = 0 \tag{25}$$

4. Special case

Now we will consider the case when the mass moment of inertia of SWCNT (I_{CNT}) is much smaller than that of buckyball ($I_{Buckyball}$). $I_{Buckyball}$ is the polar mass moment of inertia of the buckyballs. This would imply $1/\Delta I\to 0$ and accordingly $\lambda\to 0$ (see Eq. (20)). In this case, we have $\tan\lambda\approx\lambda$, which leads to a simple relation for nonlocal torsional resonant frequency as

$$\lambda^2 = (1/\Delta I) \tag{26}$$

The term λ is a function of nonlocal parameter, and is defined in Eq. (15).

Using Eq. (15), explicit nonlocal torsional frequency as a function of mass moment of inertia ratio ΔI and nonlocal parameter is evaluated as

$$\Omega_R = \sqrt{\left(\frac{1}{\Delta I}\right)\Big/\left[1+\left(\frac{e_0a}{L}\right)^2\left(\frac{1}{\Delta I}\right)\right]} \tag{27}$$

A better assumption of Eq. (27) can be found assuming

$$\tan\lambda = \lambda + \lambda^3/3 \tag{28}$$

Using Eqs. (15) and (28), we can have explicit relation for nonlocal frequency as

$$\Omega_R = \sqrt{\left(\frac{1}{\Delta I}\right)\Big/\left[1+\frac{1}{3}\left(\frac{1}{\Delta I}\right)+\left(\frac{e_0a}{L}\right)^2\left(\frac{1}{\Delta I}\right)\right]} \tag{29}$$

This expression is similar to the Rayleigh nonlocal frequency relation as described in Ref. [29]. In the next section we analyze the torsional frequency behavior due to added buckyballs and nonlocal effect.

5. Results and discussion

The nonlocal effects and the influence of attached buckyballs on the torsional vibration of carbon nanotubes are presented in this section. The derived expressions for torsional vibration are

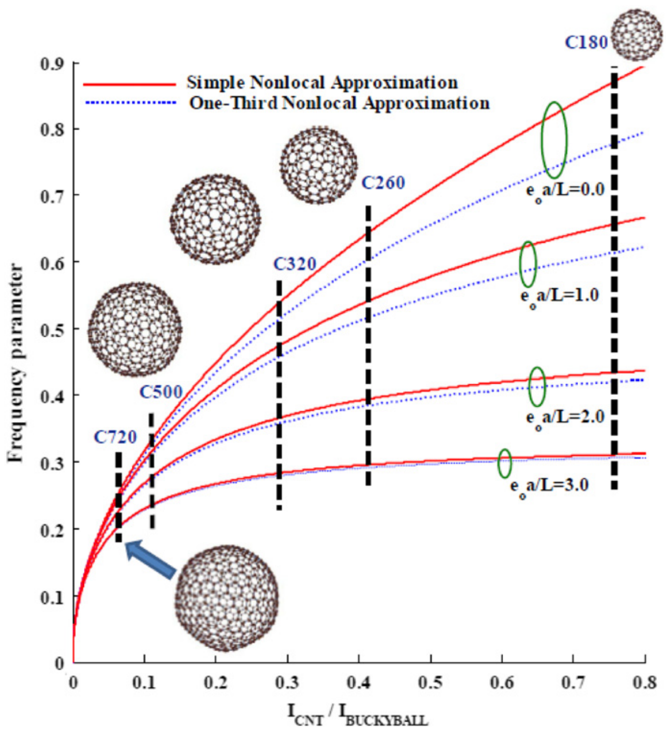

Fig. 2. Variation in torsional frequency parameter with mass moment of inertia ratio for carbon nanotube–buckyball system when the mass of buckyball is larger than carbon nanotube.

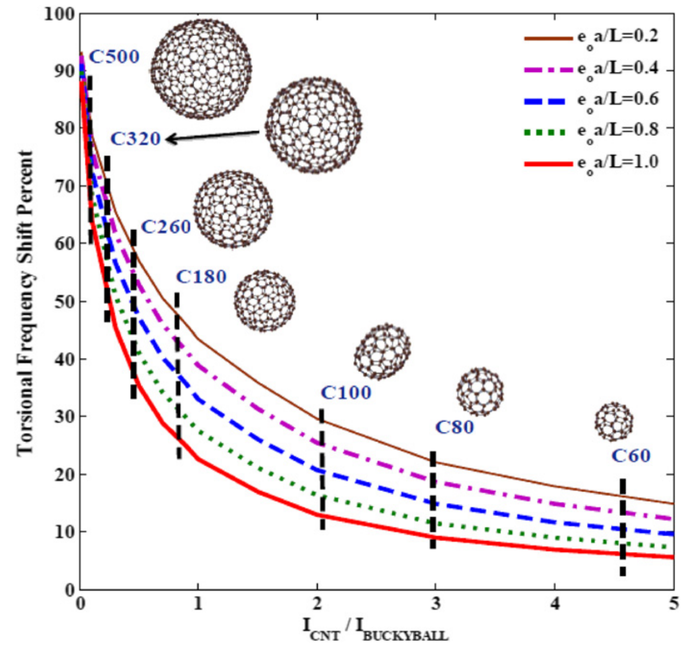

Fig. 3. Effect of mass moment of inertia ratio on torsional frequency shift percent (TFSP) of the vibrating system for various dimensionless nonlocal parameters.

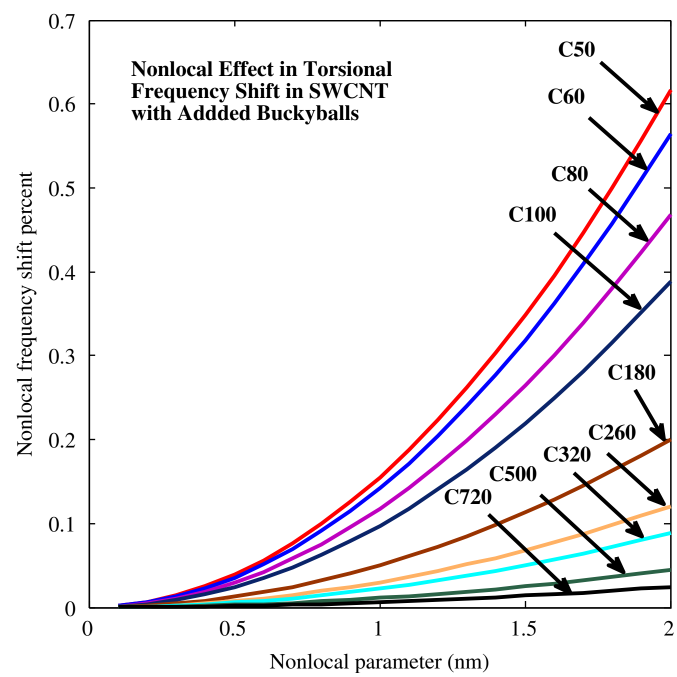

Fig. 4. Effect of nonlocal parameter on nonlocal torsional frequency shift percent (NFSP) parameter for vibrating system with different standard carbon buckyballs.

discussed. An armchair SWCNT (5, 5) of length $L=24.4$ nm, density $\rho=9.517\times10^3$ kg/m^3, and thickness $h=0.08$ nm is considered [31]. Fig. 2 shows the variation in nondimensional nonlocal torsional frequency Ω against the mass moment of inertia ratio of the vibrating system, $1/\Delta I$, for the case of I_{CNT} smaller than $I_{Buckyball}$. The range of ratio is taken as $0<(1/\Delta I)<0.8$. As $(1/\Delta I)$ increases, the frequency parameter Ω increases. The increase in Ω is due to the increase in shear rigidity of the vibrating system. When the value of the nonlocal parameter (e_0a/L) is raised, the torsional frequency parameter Ω decreases for the entire range of mass ratio $(1/\Delta I)$ considered. This reduction in frequency parameter is due to the incorporation of small-scale effects. Further it is noticed that the two approximate assumptions (Eqs. (27) and (29)) impart similar results with increase in nonlocal parameter.

Now we consider the arbitrary mass moment of inertia ratios of the vibrating system. The transcendental equation for torsional vibration (Eq. (20)) is computed numerically. We define the torsional frequency shift percent as (TFSP)

$$\mathrm{TFSP}=100\times\frac{\Omega_{No\ buckyball}-\Omega_{with\ buckyball}}{\Omega_{No\ buckyball}} \tag{30}$$

The term TFSP reflects the deviation in torsional frequency values of the vibrating system from the SWCNT without buckyballs. TFSP is plotted for various mass moment of inertia ratios $1/\Delta I$ and is illustrated in Fig. 3. One can see that when $1/\Delta I\to0$, $(I_{Buckyball}\to\infty)$TFSP is 100%. Torsional frequency shift of the vibrating system increases with increase in the attached nanomass (buckyballs) with respect to the mass of SWCNT. This implies that attaching different buckyballs at the tip, the torsional resonance frequency can be tuned accordingly and can be used as tunable nanoresonator. As the mass of SWCNT increases, the TFSP decreases. This decreasing trend is much influenced (reduced) by increasing dimensionless nonlocal parameter (e_0a/L).

Now we consider the nonlocal effects on vibrating SWCNT-attached-buckyballs. Nonlocal frequency shift percent (NFSP) under torsional vibration is computed for SWCNT attached with various standard buckyballs. NFSP represents the shift in frequency in vibrating nanostructures when the nonlocal effects are ignored.

Torsional nonlocal frequency shift percent is defined as

$$\mathrm{NFSP}=100\times\frac{\Omega_{Local}-\Omega_{Nonlocal}}{\Omega_{local}} \tag{31}$$

Nonlocal frequency shift percent (NFSP) is plotted against dimensional nonlocal parameter for SWCNT attached with various standard buckyballs (Fig. 4). Dimensional nonlocal

Table 1
Ratio (ΔI) of SWCNT (5, 5) and buckyballs (spherical fullerenes).

Buckyballs	C_{50}	C_{60}	C_{80}	C_{100}	C_{180}	C_{260}	C_{320}	C_{500}	C_{720}
ΔI	0.1564	0.2119	0.3422	0.4964	1.3221	2.4403	3.4493	7.2572	13.3261

parameter, $e_0a=0-2.0$ nm [11], is assumed. Here we consider the standard buckyballs. Different carbon buckyballs considered are C_{50}, C_{60}, C_{80}, C_{100}, C_{180}, C_{260}, C_{320}, C_{500} and C_{720}. The mass moment of inertia of these buckyballs is obtained using Eq. (22). The mass density of buckyballs is assumed to be 1720 kg/m^3. Vibrating systems are assumed by attaching different buckyballs at the tip of SWCNT. A SWCNT (5, 5) for length $L=24.4$ nm is considered. The radius of SWCNT is determined as $R=0.246/2\pi\sqrt{n^2+nm+m^2}$. The practical mass moment of inertia ratios ΔI of the vibrating system with different standard buckyballs are listed in Table 1.

From Fig. 4 it is found that increasing the dimensional nonlocal parameter increases the nonlocal frequency shift. Based on the nonlocal elasticity theory, long-range interactions are taken into account in the analysis that makes the vibrating system stiffer. This trend is obvious when the attached buckyballs are small as compared with the SWCNTs. The figure shows that with lighter buckyballs (viz. C_{50}, C_{60} and C_{80}) the nonlocal effects on torsional NFSP are more pronounced compared to SWCNT with heavier buckyballs (viz. C_{320}, C_{500} and C_{720}). This is similar to the behavior in longitudinal vibration of SWCNT with attached buckyballs [29].

6. Conclusion

The torsional vibration of SWCNTs with added buckyballs at one end and the other end fixed is studied by considering nonlocal effects on the nanoresonators. In the special case when the mass moment of inertia of the attached buckyball is much larger than that of the SWCNTs, explicit expressions relating torsional nonlocal frequencies and mass moment of inertia ratio are obtained. A closed-form nonlocal transcendental equation is derived for general cases. We found that torsional resonant frequency shift of the vibrating system increases sensitively with the growing mass (moment of inertia) of the buckyballs. Higher frequency shift can also be achieved by raising the value of nonlocal parameter. Such an effect of nonlocal parameter becomes more pronounced for the nanoresonators with smaller buckyballs. Indeed the outcomes of this study provide efficient mathematical modeling tool for the vibration of the nanostructures and bring in an in-depth understanding of nonlocal effects on the carbon nanotube–buckyball nanoresonators.

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