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Nonlinear vibrations and energy distribution of Single-Walled Carbon Nanotubes

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Abstract
The nonlinear vibrations of Single-Walled Carbon Nanotubes are analysed. The Sanders-Koiter elastic shell theory is applied in order to obtain the elastic strain energy and kinetic energy. The carbon nanotube deformation is described in terms of longitudinal, circumferential and radial displacement fields. The theory considers geometric nonlinearities due to large amplitude of vibration. The displacement fields are expanded by means of a double series based on harmonic functions for the circumferential variable and Chebyshev polynomials for the longitudinal variable. The Rayleigh-Ritz method is applied in order to obtain approximate natural frequencies and mode shapes. Free boundary conditions are considered. In the nonlinear analysis, the three displacement fields are re-expanded by using approximate eigenfunctions. An energy approach based on the Lagrange equations is considered in order to obtain a set of nonlinear ordinary differential equations. The energy distribution of the system is studied by considering combinations of different vibration modes. The effect of the conjugate modes participation on the energy distribution is analysed.

Keywords
Nonlinear vibrations, energy distribution, carbon nanotubes

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Introduction

Carbon Nanotubes were discovered in 1991 by Iijima [1], who first analysed the synthesis of molecular carbon structures in the form of fullerenes and then reported the preparation of a new type of finite carbon structure, the carbon nanotubes, described as helical microtubules of graphitic carbon.

Rao et al. [2] studied the vibrations of SWNTs by using Raman scattering experimental techniques with laser excitation wavelengths in the range of the nanometers. They observed numerous Raman peaks, which correspond to vibrational modes of the nanotubes.

Gupta et al. [3] simulated the mechanical behaviour of SWNTs with free edges by using the molecular dynamics potential. They considered the effect of the chirality and geometry on the natural frequencies of the longitudinal, torsional and inextensional modes of vibration.

Arghavan and Singh [4] carried out a numerical study on the free and forced vibrations of SWNTs by considering the FE method. They analysed different boundary conditions, obtaining the natural frequencies and mode shapes, time histories and spectra of axial, bending and torsional modes.

Wang et al. [5] examined the applicability and limitations of different simplified models of elastic cylindrical shells for general cases of static buckling and free vibrations of carbon nanotubes. They considered the Flugge, Donnell thin shell and Donnell shallow shell models.

Strozzi et al. [6] analysed the linear vibrations of SWNTs for various boundary conditions in the framework of the Sanders-Koiter thin shell theory. They analysed several types of nanotubes by varying aspect ratio and chirality in a wide range of the natural frequency spectrum.

In the present paper, the nonlinear vibrations of SWNTs are analysed. The Sanders-Koiter thin shell theory is applied. The displacement fields are expanded by means of a double series based on harmonic functions for the circumferential variable and Chebyshev polynomials for the longitudinal variable. The Rayleigh-Ritz method is applied to obtain approximate natural frequencies and mode shapes. Free boundary conditions are considered. In the nonlinear analysis, the three displacement fields are re-expanded by using approximate eigenfunctions. The Lagrange equations are considered to obtain a set of nonlinear ordinary differential equations. The total energy distribution is studied by considering different combined modes. The effect of the conjugate modes participation is analysed.

1. Elastic strain energy

The nondimensional elastic strain energy $\tilde{U}$ of a cylindrical shell, by neglecting the transverse normal stress σ_z (plane stress hypothesis) and the transverse shear strains γ_{xz}, $\gamma_{\theta z}$, is written as

$$\begin{aligned}\tilde{U} = &\frac{1}{2}\int_0^1\int_0^{2\pi}\left(\tilde{\varepsilon}_{x,0}^2+\tilde{\varepsilon}_{\theta,0}^2+2\nu\tilde{\varepsilon}_{x,0}\tilde{\varepsilon}_{\theta,0}+\frac{(1-\nu)}{2}\tilde{\gamma}_{x\theta,0}^2\right)d\theta d\eta \\ &+\frac{1}{2}\frac{\beta^2}{12}\int_0^1\int_0^{2\pi}\left(\tilde{k}_x^2+\tilde{k}_\theta^2+2\nu\tilde{k}_x\tilde{k}_\theta+\frac{(1-\nu)}{2}\tilde{k}_{x\theta}^2\right)d\theta d\eta\end{aligned} \tag{1}$$

where ($\tilde{\varepsilon}_{x,0}$, $\tilde{\varepsilon}_{\theta,0}$, $\tilde{\gamma}_{x\theta,0}$) are the nondimensional middle surface strains, ($\tilde{k}_x$, $\tilde{k}_\theta$, $\tilde{k}_{x\theta}$) represent the nondimensional middle surface changes in curvature and torsion, with ($\eta = x / L$) and ($\beta = h / L$).

2. Kinetic energy

The nondimensional kinetic energy $\tilde{T}$ of a cylindrical shell (rotary inertia neglected) is given by

$$\tilde{T} = \frac{1}{2}\int_0^1\int_0^{2\pi}(\tilde{u}'^2+\tilde{v}'^2+\tilde{w}'^2)d\theta d\eta = \frac{1}{2}\int_0^1\int_0^{2\pi}\left[\left(\frac{d\tilde{u}}{d\tau}\right)^2+\left(\frac{d\tilde{v}}{d\tau}\right)^2+\left(\frac{d\tilde{w}}{d\tau}\right)^2\right]d\theta d\eta \tag{2}$$

where ($\tilde{u}$, $\tilde{v}$, $\tilde{w}$) are the nondimensional displacement fields, ($\tilde{u}'$, $\tilde{v}'$, $\tilde{w}'$) denote the nondimensional velocity fields and τ is the nondimensional time variable obtained by introducing a reference natural frequency ω_0.

2. Linear vibration analysis

A modal vibration can be written in the form

$$\tilde{u}(\eta,\theta,\tau)=\tilde{U}(\eta,\theta)\varphi(\tau) \qquad \tilde{v}(\eta,\theta,\tau)=\tilde{V}(\eta,\theta)\varphi(\tau) \qquad \tilde{w}(\eta,\theta,\tau)=\tilde{W}(\eta,\theta)\varphi(\tau) \tag{3}$$

where $\tilde{U}(\eta,\theta)$, $\tilde{V}(\eta,\theta)$, $\tilde{W}(\eta,\theta)$ describe the mode shape and $\varphi(\tau)$ is the nondimensional time law.

The mode shape is expanded by means of a double series in terms Chebyshev polynomials $T_m^*(\eta)$ in the axial direction and harmonic functions (cos $n\theta$, sin $n\theta$) in the circumferential direction

$$\tilde{U}(\eta,\theta)=\sum_{m=0}^{M_u}\sum_{n=0}^{N}\tilde{U}_{m,n}T_m^*(\eta)\cos n\theta \tag{4}$$

$$\tilde{V}(\eta,\theta)=\sum_{m=0}^{M_v}\sum_{n=0}^{N}\tilde{V}_{m,n}T_m^*(\eta)\sin n\theta \tag{5}$$

$$\tilde{W}(\eta,\theta)=\sum_{m=0}^{M_w}\sum_{n=0}^{N}\tilde{W}_{m,n}T_m^*(\eta)\cos n\theta \tag{6}$$

where $T_m^* = T_m\,(2\eta - 1)$, m is the polynomials degree and n denotes the number of nodal diameters.

3. Nonlinear vibration analysis

The displacement fields $\tilde{u}(\eta,\theta,\tau)$, $\tilde{v}(\eta,\theta,\tau)$, $\tilde{w}(\eta,\theta,\tau)$ are expanded by using both the linear mode shapes $\tilde{U}(\eta,\theta)$, $\tilde{V}(\eta,\theta)$, $\tilde{W}(\eta,\theta)$ obtained in the previous linear analysis and the conjugate mode shapes $\tilde{U}_c(\eta,\theta)$, $\tilde{V}_c(\eta,\theta)$, $\tilde{W}_c(\eta,\theta)$ in the following form

$$\begin{aligned}
\tilde{u}(\eta,\theta,\tau) &= \sum_{j=1}^{N_u}\sum_{n=1}^{N}\left[\tilde{U}^{(j,n)}(\eta,\theta)\varphi_{u,j,n}(\tau)+\tilde{U}_c^{(j,n)}(\eta,\theta)\varphi_{u,j,n,c}(\tau)\right]\\
\tilde{v}(\eta,\theta,\tau) &= \sum_{j=1}^{N_v}\sum_{n=1}^{N}\left[\tilde{V}^{(j,n)}(\eta,\theta)\varphi_{v,j,n}(\tau)+\tilde{V}_c^{(j,n)}(\eta,\theta)\varphi_{v,j,n,c}(\tau)\right]\\
\tilde{w}(\eta,\theta,\tau) &= \sum_{j=1}^{N_w}\sum_{n=1}^{N}\left[\tilde{W}^{(j,n)}(\eta,\theta)\varphi_{w,j,n}(\tau)+\tilde{W}_c^{(j,n)}(\eta,\theta)\varphi_{w,j,n,c}(\tau)\right]
\end{aligned} \tag{7}$$

The Lagrange equations of motion for free vibrations are expressed in the following form

$$\frac{d}{d\tau}\left(\frac{\partial\tilde{L}}{\partial\dot{\tilde{q}}_i}\right)-\frac{\partial\tilde{L}}{\partial\tilde{q}_i}=0 \qquad i\in[1,N_{\max}] \qquad (\tilde{L}=\tilde{T}-\tilde{U}) \tag{8}$$

where the nondimensional modal coordinates $\tilde{q}_i$ are ordered in a vector $\tilde{q}(\tau)$ = [..., $\varphi_{u,j,n}$, $\varphi_{u,j,n,c}$, $\varphi_{v,j,n}$, $\varphi_{v,j,n,c}$, $\varphi_{w,j,n}$, $\varphi_{w,j,n,c}$, ...] and the maximum number of degrees of freedom N_{max} depends on the number of modes considered in expansions (7).

Using the Lagrange equations (8), a set of nonlinear ordinary differential equations is obtained; such system is then solved by using numerical methods.

4. Numeric results

In order to analyse the discrete molecular carbon nanotube as a continuum thin shell, equivalent mechanical parameters (Young's modulus, Poisson's ratio, mass density, wall thickness) must be considered. These parameters are not dependent from the CNT diameter (no size effect). The carbon nanotube described in Table 1 is considered for the following computations.

Table 1. Effective and equivalent parameters of the Single-Walled Carbon Nanotube

Effective thickness h_0 (nm)	0.10 ÷ 0.15
Equivalent thickness h (nm)	0.066
Effective Young's modulus E_0 (TPa)	1.0 ÷ 2.0
Equivalent Young's modulus E (TPa)	5.5
Effective Poisson's ratio ν_0	0.12 ÷ 0.28
Equivalent Poisson's ratio ν	0.19
Surface density of graphite σ (kg/m^2)	7.718×10^{-7}
Equivalent mass density ρ (kg/m^3)	11700

The present model is validated with molecular dynamics data available in the literature [3]; the results reported in Table 2 show that the model is accurate and the equivalent parameters are correct.

Table 2. Natural frequencies of the radial breathing mode (j = 0, n = 0): comparisons between the Sanders-Koiter theory (SKT) and the Molecular Dynamics Simulations (MDS).

Natural frequency (THz)			**Difference %**
(r, s)	SKT - Present model	MDS - Ref. [3]	
(10, 0)	8.966	8.718	2.84
(6, 6)	8.636	8.348	3.45
(12, 0)	7.478	7.272	2.83
(7, 7)	7.399	7.166	3.25
(8, 8)	6.473	6.275	3.15
(14, 0)	6.414	6.235	2.87
(16, 0)	5.606	5.455	2.77
(10, 10)	5.184	5.026	3.14
(18, 0)	4.985	4.850	2.78
(20, 0)	4.489	4.364	2.86

In Figures 1(a-f), three mode shapes of a free-free carbon nanotube are presented, such modes are considered for the development of the semi-analytic nonlinear model of the carbon nanotube in the re-expansion of Equation (7). In Figures 2-4, the total vibration energy distribution is represented, where the nanotube is unwrapped on a plane in order to allow the energy representation. The damping is not considered here, so the total energy is constant (the integral of the density over the surface).

The sequence of Figures 2(a-f) shows the distribution of the total energy density [Jm^{-2}] in the linear field during a time period corresponding to the natural frequency of the fundamental mode. The analysis of the total energy distribution over the shell shows a periodicity along the circumferential direction. This is expected as in this preliminary linear analysis no conjugate modes are present. The energy is distributed symmetrically along the longitudinal direction because we are combining the two symmetric modes (0,2) and (2,2).

The sequence of Figures 3(a-f) shows the distribution of the total energy density [Jm^{-2}] in the nonlinear field for the two combined modes (0,2) and (2,2). Comparing linear and nonlinear analyses (with same initial conditions) we obtain that, due to the nonlinearity, the energy distribution changes dramatically evolving in a complex pattern with absence of periodicity.

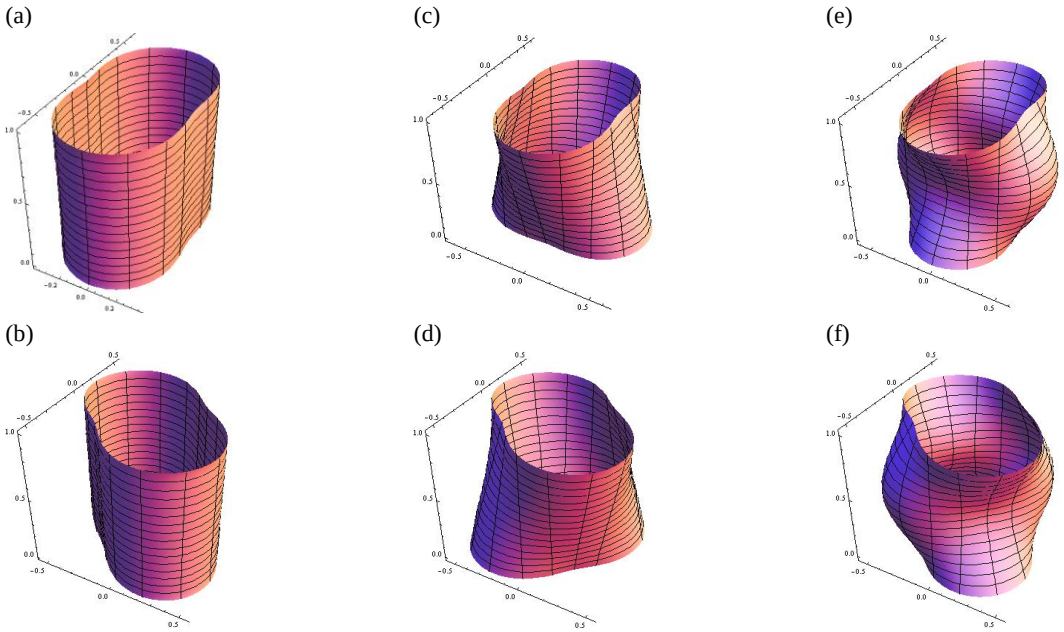

Figure 1. Mode shapes of the SWNT (r = 10, s = 0, L = 10.0 nm). Equivalent parameters of Table 1. (a),(b) Conjugate modes (0,2). (c),(d) Conjugate modes (1,2). (e),(f) Conjugate modes (2,2).

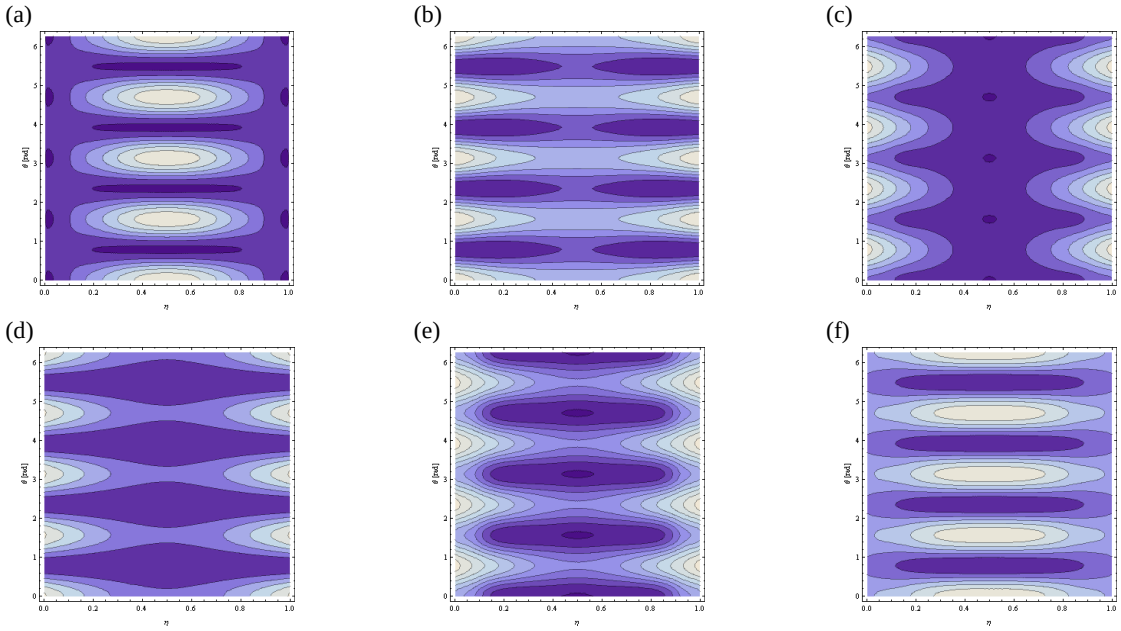

Figure 2. Contour plots of the total energy distribution $\tilde{E}(\eta, \theta, \tau)$. Linear vibration analysis. Combined modes (0,2) and (2,2). (a) $\tau = 4.90$. (b) $\tau = 6.40$. (c) $\tau = 7.60$. (d) $\tau = 8.20$. (e) $\tau = 9.40$. (f) $\tau = 10.60$.

The sequence of Figures 4(a-f) shows the total energy density [Jm^{-2}] in the nonlinear field for the two conjugate modes (1,2). The periodicity along the circumferential direction is now lost due to the presence of the conjugate modes and the nonlinearity. The participation of both conjugate modes gives rise to a travelling wave moving circumferentially around the shell. The initial conditions on the conjugate modes are different, one of them is activated and the second one is slightly perturbed, i.e., an infinitesimal initial energy is provided; after a suitably long time period the conjugate mode having infinitesimal initial energy is activated and it vibrates with large amplitude, this is due to an internal transfer of energy probably due to the internal resonance (1:1). The activation of the second conjugate mode implies that the energy distribution on the shell surface is completely different with respect to the linear model.

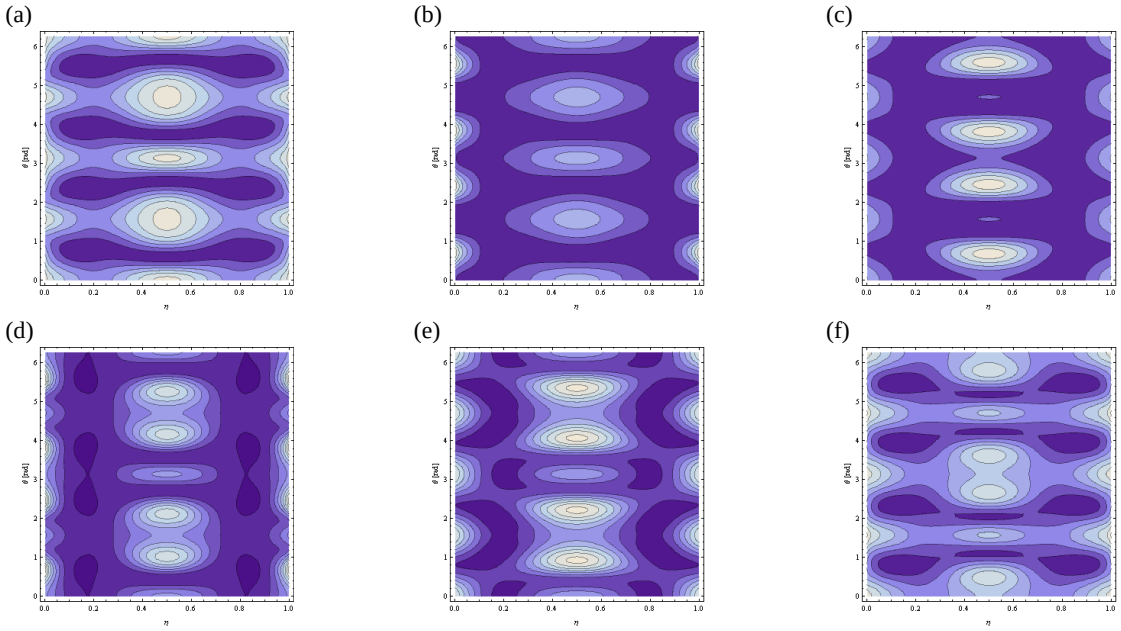

Figure 3. Contour plots of the total energy distribution $\tilde{E}(\eta, \theta, \tau)$. Nonlinear analysis. Combined modes (0,2), (2,2). (a) $\tau = 10.88$. (b) $\tau = 10.91$. (c) $\tau = 11.00$. (d) $\tau = 11.15$. (e) $\tau = 11.39$. (f) $\tau = 11.54$.

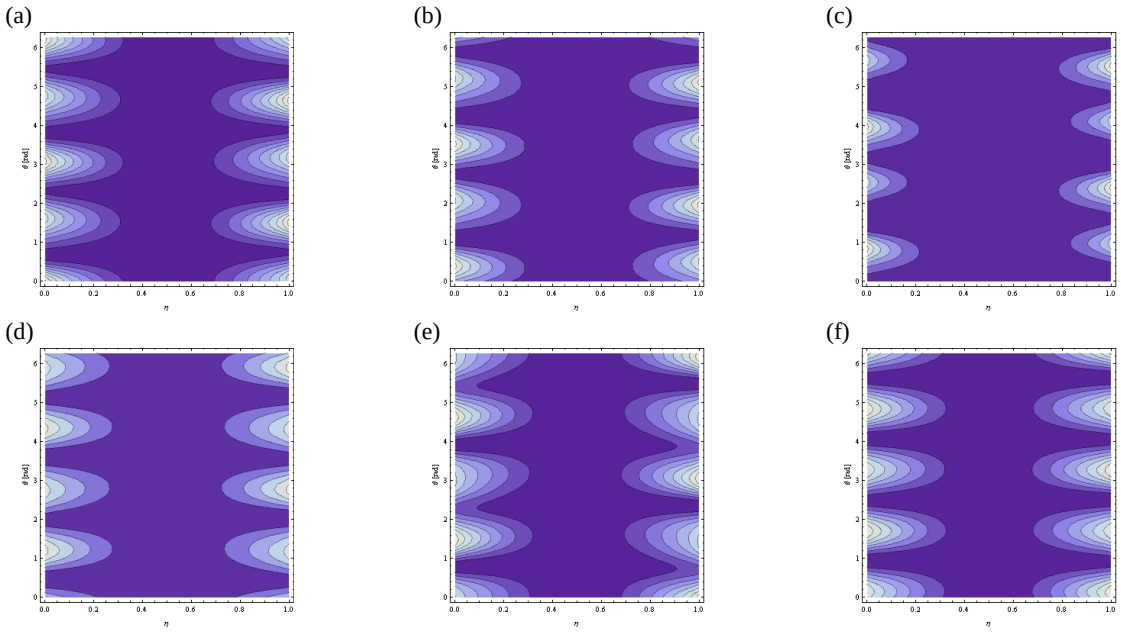

Figure 4. Contour plots of the total energy distribution $\tilde{E}(\eta, \theta, \tau)$. Nonlinear analysis. Conjugate modes (1,2). (a) $\tau = 7.68$. (b) $\tau = 7.72$. (c) $\tau = 7.76$. (d) $\tau = 7.92$. (e) $\tau = 8.06$. (f) $\tau = 8.08$.

Conclusions

The nonlinear vibrations of SWNTs are studied. Equivalent parameters, which allow to analyse the discrete carbon nanotube as a continuum thin shell, are considered. The Sanders-Koiter elastic shell theory is applied in order to obtain the elastic strain energy and kinetic energy. The Rayleigh-Ritz method is applied in order to obtain approximate natural frequencies and mode shapes. The present model is validated in linear field with molecular dynamics data available in the literature. An energy approach based on the Lagrange equations is considered in order to obtain a set of nonlinear ordinary differential equations. The total energy distribution is analysed, where the nanotube is unwrapped on a plane in order to allow the energy representation. The energy distribution in linear and nonlinear field with the same initial conditions is compared. The nonlinear energy distribution changes dramatically evolving in a complex pattern with absence of periodicity. The participation of conjugate modes gives rise to an energy transfer between the two conjugate modes and nonstationary response.

References

[1] Iijima S. Helical microtubules of graphitic carbon. *Nature*, 354, pp. 56-58, 1991.
[2] Rao AM, Richter E, Bandow S, Chase B, Eklund PC, Williams KA, Fang S, Subbaswamy KR, Menon M, Thess A, Smalley RE, Dresselhaus G and Dresselhaus MS. Diameter-Selective Raman Scattering from Vibrational Modes in Carbon Nanotubes. *Science*, 275, pp. 187-191, 1997.
[3] Gupta SS, Bosco FG and Batra RC. Wall thickness and elastic moduli of single-walled carbon nanotubes from frequencies of axial, torsional and inextensional modes of vibration. *Computational Materials Science*, 47, pp. 1049-1059, 2012.
[4] Arghavan S and Singh AV. On the vibrations of single-walled carbon nanotubes. *Journal of Sound and Vibration*, 330, pp. 3102-3122, 2011.
[5] Wang CY, Ru CQ and Mioduchowski A. Applicability and Limitations of Simplified Elastic Shell Equations for Carbon Nanotubes. *Journal of Applied Mechanics*, 71, pp. 622-631, 2004.
[6] Strozzi M, Manevitch LI, Pellicano F, Smirnov VV and Shepelev DS. Low-frequency linear vibrations of Single-Walled Carbon Nanotubes: analytical and numerical models. *Journal of Sound and Vibration* (paper submitted).