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Procedia Engineering 199 (2017) 705–710

Procedia Engineering

www.elsevier.com/locate/procedia

X International Conference on Structural Dynamics, EURODYN 2017

Nonlinear optical vibrations of single-walled carbon nanotubes.

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Abstract

We demonstrate a new specific phenomenon of the long-time resonant energy exchange in carbon nanotubes (CNTs), which is realized by two types of optical vibrations, the Circumferential Flexure Mode (CFM) and the Radial Breathing Mode (RBM). We show that the modified nonlinear Schrdinger equation, obtained in the framework of the nonlinear theory of elastic thin shells, allows us to describe the nonlinear dynamics of CNTs for specified frequency bands. Comparative analysis of the oscillations of the CFM and RBM branches shows the qualitative difference of nonlinear effects for these branches. While the nonlinear resonant interaction of the low-frequency modes in the CFM branch leads to energy capture in some domains of the CNT, the same interaction in the RBM branch does not demonstrate any tendency for energy localization. The reason lies in the distinction in the nonlinear terms in the equations of motion. While CFMs are characterized by soft polynomial nonlinearity, RBM dynamics is characterized by hard gradient nonlinearity. Moreover, in contrast to the CFM, the importance of nonlinearity in the case of RBM oscillations decreases as the length to radius ratio increases. Numerical integration of the equations of thin shell theory confirms the results of the analytical study.

Peer-review under responsibility of the organizing committee of EURODYN 2017.

Keywords: carbon nanotubes; nonlinear vibrations; energy exchange; energy localization

1. Introduction

The nonlinear dynamics of CNTs is an important application of the various processes studied in physics, chemistry, material science, and biophysics. Presently, theoretical research is conducted either in the framework of the atomistic approach or is based on the dynamics of continuum systems. The last approach allows the application of the well-developed methods of the theory of thin elastic shells. However, the results of the analysis have to comply with the microscopic theory of CNTs. There is one more reason to apply the theory of elastic shells to the dynamics of CNTs. It is well known that defectless CNTs can reversibly withstand large deformations without the appearance of any plasticity.

In this work we will shortly discuss specific phenomenon, such as the interaction of linear optical-type vibrations in the framework of the theory of elastic thin shells studied by Sanders and Koiter. We shall review the results of mode coupling for two types of vibrations specific to thin shells (see fig. 1 and its caption). The first type corresponds

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1877-7058
Peer-review under responsibility of the organizing committee of EURODYN 2017.
10.1016/j.proeng.2017.09.011

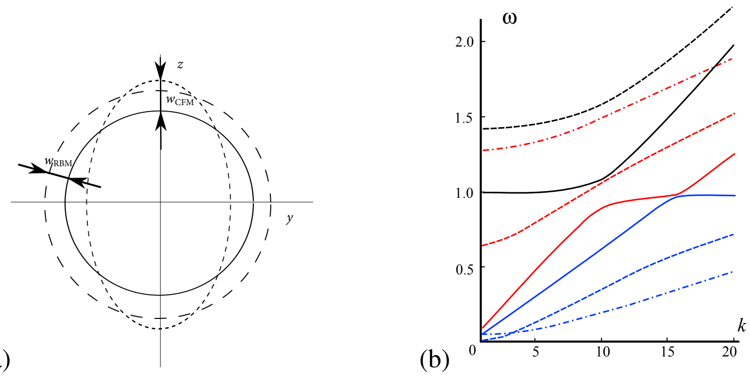

Fig. 1. (a) The specific changes of lateral section of a CNT during the radial breathing (long-dashes) and circumferential flexure (dashes) oscillations. The solid curves show the undistorted profile of the CNT. The arrows show the specific radial displacements which occur during the radial breathing (w_{RBM}) and circumferential flexure (w_{CFM}) oscillations. (b) The vibration spectrum according to the exact Sanders-Koiter thin shell theory for the CNT with aspect ratio $L/R = 30$ under the periodic boundary conditions: solid curves correspond to the circumferential wave number $n = 0$, dashed curves to $n = 1$, and dash-dotted curves - to $n = 2$. All the frequencies ω are dimensionless, the parameter k denotes the number of longitudinal half-waves along the CNT.

to the axisymmetric deformations of CNTs and is often called the Radial Breathing Mode (RBM). The second one is related to the asymmetric deformations of CNTs' cross-section. Since a CNT's axis does not deflect from a straight line, these oscillations are identified as the Circumferential Flexure Mode (CFM). Both of these modes are specified by a gap in the long wavelength edge of the spectrum, therefore they belong to the optical type. The values of the gaps are determined by the rigidity of the graphen sheet under uniaxial deformation (RBM) and the bending modulus of the sheet (CFM). Therefore, these values are different. However, a common feature of the optical-type vibrational branches is the crowding of frequencies near the long wave edge of the spectrum. Thus, the possibility of the resonant interaction of nonlinear normal modes (NNMs) appears. Nevertheless, the result of such interactions depends strongly on the specified mode.

Because the model has been described in detail earlier [1–3] we will discuss below only the main hypotheses and results of the analysis.

2. The background

A key problem in the study of CNT nonlinear dynamics dominated by certain types of vibrations is to construct an adequately reduced model, which takes into account the main features of CNT deformations.

We will start our study with the dimensionless energy of the elastic deformation of a CNT, which can be written as follows:

$$E_{el} = \frac{1}{2}\int_0^1\int_0^{2\pi}\left(\varepsilon_\xi^2 + \varepsilon_\varphi^2 + 2\nu\varepsilon_\xi\varepsilon_\varphi + \frac{1-\nu}{2}\varepsilon_{\xi\varphi}^2\right)d\xi d\varphi + +\frac{\beta^2}{24}\int_0^1\int_0^{2\pi}\left(\kappa_\xi^2 + \kappa_\varphi^2 + 2\nu\kappa_\xi\kappa_\varphi + \frac{1-\nu}{2}\kappa_{\xi\varphi}^2\right)d\xi d\varphi. \tag{1}$$

where ε_ξ, ε_φ and $\varepsilon_{\xi\varphi}$ are the longitudinal, circumferential and shear deformations, and κ_ξ, κ_φ and $\kappa_{\xi\varphi}$ are the longitudinal curvature, circumferential curvature, and torsion, respectively.

The dimensionless energy and time variables are measured in the units $E_0 = YRLh/(1-\nu^2)$ and $t_0 = 1/\sqrt{Y/\rho R^2(1-\nu^2)}$, respectively. Here Y is the Young modulus of a graphene sheet, ρ - its mass density, ν - the Poisson ratio of the CNT; R, L and h are the CNT's radius, length and wall thickness. Two dimensionless geometric parameters characterize a CNT: the inverse aspect ratio $\alpha = R/L$, and the relative thickness of the effective shell $\beta = h/R$.

The Sanders-Koiter approximation of a defectless thin shell allows us to write the nonlinear deformations (ε) and curvatures (κ) in the following form

$$\begin{aligned}
&\varepsilon_\xi = \alpha\frac{\partial u}{\partial\xi} + \frac{\alpha^2}{2}\left(\frac{\partial w}{\partial\xi}\right)^2 + \frac{1}{8}\left(\alpha\frac{\partial v}{\partial\xi} - \frac{\partial u}{\partial\varphi}\right)^2, \quad \varepsilon_\varphi = \frac{\partial v}{\partial\varphi} + w + \frac{1}{2}\left(\frac{\partial w}{\partial\varphi} - v\right)^2 + \frac{1}{8}\left(\frac{\partial u}{\partial\varphi} - \alpha\frac{\partial v}{\partial\xi}\right)^2,\\
&\varepsilon_{\xi\varphi} = \frac{\partial u}{\partial\varphi} + \alpha\frac{\partial v}{\partial\xi} + \alpha\frac{\partial w}{\partial\xi}\left(\frac{\partial w}{\partial\varphi} - v\right)
\end{aligned} \tag{2}$$

$$\kappa_\xi = -\alpha^2\beta\frac{\partial^2 w}{\partial\xi^2}, \quad \kappa_\varphi = \beta\left(\frac{\partial v}{\partial\varphi} - \frac{\partial^2 w}{\partial\varphi^2}\right), \quad \kappa_{\xi\varphi} = \beta\left(-2\alpha\frac{\partial^2 w}{\partial\xi\partial\varphi} + \frac{3\alpha}{2}\frac{\partial v}{\partial\xi} - \frac{1}{2}\frac{\partial u}{\partial\varphi}\right). \tag{3}$$

where u, v and w are dimensionless (in the units of the CNT's radius R) longitudinal, tangential and radial displacements, respectively; ξ is a dimensionless (in the units of the CNT's length L) coordinate along the CNT axis; φ is the circumferential angle.

Introducing the applicable physical hypotheses we will reduce the full set of dynamical equations to an analytically solvable model.

3. Radial breathing mode

In this section we will consider radial breathing oscillations. Taking into account that RBMs represent the axisymmetrical mode, we can conclude that for the azimuthal angle φ the respective azimuthal wave number n equals 0 and the tangential displacement v equals 0. Under this assumption the dispersive relation of the linearized problem can be obtained as follows:

$$\omega^2 = \frac{1}{2}\left(1 + \alpha^2 k^2 + \sqrt{(1-\alpha^2k^2)^2 + 4\alpha^2\nu^2k^2}\right), \tag{4}$$

where k is the longitudinal wave number (see fig. 1(b)). The respective eigenvector

$$(u, w) = (-\alpha\nu k, 1) \tag{5}$$

shows the relationship between the longitudinal and radial components of the displacement field. Taking into account the expression (5) we can exclude the longitudinal displacement u and write the equation for radial displacement w as follows:

$$\frac{\partial^2 w}{\partial\tau^2} + w - \alpha^2\nu^2\frac{\partial^2 w}{\partial\xi^2} - \alpha^2\nu\left(\frac{1}{2}\left(\frac{\partial w}{\partial\xi}\right)^2 + w\frac{\partial^2 w}{\partial\xi^2}\right) + \alpha^4\left(\frac{1}{12}\beta^2\frac{\partial^4 w}{\partial\xi^4} + \nu\frac{\partial}{\partial\xi}\left(\frac{\partial w}{\partial\xi}\frac{\partial^2 w}{\partial\xi^2}\right) - \frac{3}{2}\left(\frac{\partial w}{\partial\xi}\right)^2\frac{\partial^2 w}{\partial\xi^2}\right) = 0 \tag{6}$$

To perform an asymptotic analysis of the long wavelength dynamics of the RB modes, it is convenient to rewrite equation (6) in complex variables $\psi = 1/\sqrt{2}\,(\partial w/\partial\tau + iw)$.

We can now show that the assumption of the smallness of the Poisson ratio $\nu < 1$ allows us to get an adequate description of the nonlinear dynamics of the RMB. Representing the variable ψ as a sum over the small parameter and performing a multi-scale expansion, we obtain the equation for the main order amplitude in the "slow" time τ_2 (see [2,3] for details):

$$i\frac{\partial\psi_0}{\partial\tau_2} - \alpha^2\frac{1}{2}\frac{\partial^2\psi_0}{\partial\xi^2} - \alpha^4\frac{3}{8}\frac{\partial}{\partial\xi}\left(\left|\frac{\partial\psi_0}{\partial\xi}\right|^2\frac{\partial\psi_0}{\partial\xi}\right) = 0. \tag{7}$$

Equation (7) admits the plane-wave solution

$$\psi_0 = A\exp\left(-i\left(\tilde{\omega}\tau_2 - k\xi\right)\right). \tag{8}$$

Equation (7) is the modified Nonlinear Schrödinger Equation (NLSE) whose nonlinearity has a positive gradient. The standard NLSE admits a localized solution. However, no localized solution of equation (7) is known. We will try to examine the possibility of energy localization while dealing with equation (7). First of all, we replace equation (7) with its modal representation, taking into account only two resonant NNMs with wave numbers k_1 and k_2.

$$\psi_0 = \chi_1(\tau_2)\sin(\pi k_1\xi) + \chi_2(\tau_2)\sin(\pi k_2\xi) \tag{9}$$

After the substitution of solution (9) into equation (7) we use the Galerkin procedure to obtain the equations for complex amplitudes χ_1 and χ_2:

$$\begin{aligned} &i\tfrac{\partial\chi_1}{\partial\tau_2} + \delta\omega_1\chi_1 - \tfrac{3\sigma_{11}}{2}|\chi_1|^2\chi_1 - \sigma_{12}\left(2|\chi_2|^2\chi_1 + \chi_2^2\chi_1^*\right) = 0 \\ &i\tfrac{\partial\chi_2}{\partial\tau_2} + \delta\omega_2\chi_2 - \tfrac{3\sigma_{22}}{2}|\chi_2|^2\chi_2 - \sigma_{12}\left(2|\chi_1|^2\chi_2 + \chi_1^2\chi_2^*\right) = 0, \end{aligned} \tag{10}$$

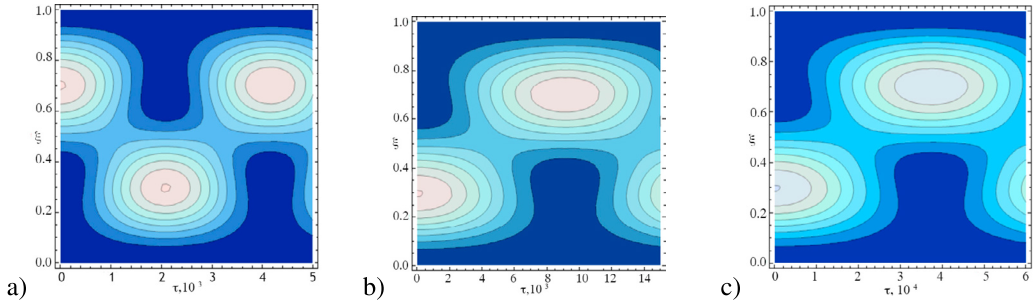

Fig. 2. (Color online) The energy exchange in the CNTs with different aspect ratios: (a) $L/R = 20$, (b) $L/R = 40$, (c) $L/R = 80$. The initial "occupation number" X equals 0.5. The dark blue and light beige areas correspond to the low and high densities of the energy, respectively.

where $\delta\omega_i = \frac{1}{2}\pi^2 k_i^2$, $(i = 1, 2)$ are the modal frequency shifts (in the "slow" time scale τ_2) from the boundary frequency $\omega_0 = 1$ of the considered branch and

$$\sigma_{ij} = \frac{3}{16}\alpha^4 k_i^2 k_j^2 \quad (i, j = 1, 2). \tag{11}$$

Equations (10) have two integrals of motion: the energy H and the "occupation numbers" X, which characterizes the excitation level of the system:

$$H = \delta\omega_1 |\chi_1|^2 + \delta\omega_2 |\chi_2|^2 - \frac{3}{4}\left(\sigma_{11}|\chi_1|^4 + \sigma_{22}|\chi_2|^4\right) - \sigma_{12}\left(2|\chi_1|^2|\chi_2|^2 + \frac{1}{2}\left(\chi_1^2\chi_2^{*2} + \chi_1^{*2}\chi_2^2\right)\right) \tag{12}$$

$$X = |\chi_1|^2 + |\chi_2|^2, \tag{13}$$

An analysis of the energy H that takes into account the additional integral X shows that the nteraction of nonlinear modes results in the energy exchange between different parts of the CNT only. The variations in the period of the energy exchange corresponding to variations in the aspect ratio of the CNT are presented in fig. 3.

4. Circumferential flexure mode

These vibrations are the lowest-frequency optical-type oscillations of the CNT (see fig. 1(b)), which correspond to the variations in the shape of the transversal cross-section without the alteration of its contour length (fig. 1(a)). The CNT axis does not deflect from a straight line, but the generatrix bends. So, such vibrations are not accompanied by any substantial circumferential and shear deformations. The circumferential wave number n equals 2. The hypotheses of smallness of circumferential and shear deformations leads to the relations:

$$\varepsilon_\varphi = 0; \quad \varepsilon_{\xi\varphi} = 0 \tag{14}$$

(These hypotheses about the relationship of widely used theories of thin shells were discussed in [4] in detail.) However, these assumptions don't imply that the displacements included in the circumferential and shear deformations are small. Contrary to linear theory, we have to take into account the axisymmetric constituent of the displacement, which accompanies oscillations with wave number n. Using relations (14) we can express the longitudinal and transversal displacements via the radial displacement:

$$\begin{aligned} &v(\xi,\tau) = -\tfrac{1}{n} w(\xi,\tau); \quad u(\xi,\tau) = -\tfrac{\alpha}{n^2}\tfrac{\partial w(\xi,\tau)}{\partial\xi} \\ &w_0(\xi,\tau) = -\tfrac{1}{4n^2}((n^2-1)^2 w^2(\xi,\tau) + \alpha^2(\tfrac{\partial W(\xi,\tau)}{\partial\xi})^2); \quad \tfrac{\partial w_0(\xi,\tau)}{\partial\xi} = -\tfrac{n^2+1}{4n^2}\alpha(\tfrac{\partial w(\xi,\tau)}{\partial\xi})^2 \end{aligned} \tag{15}$$

Omitting the calculations, the final equation of motion in terms of radial displacement $w(\xi, t)$ have the form:

$$\frac{\partial^2 w}{\partial\tau^2} + \omega_0^2 w - \mu\frac{\partial^2 W}{\partial\xi^2} - \gamma\frac{\partial^4 w}{\partial\xi^2\partial\tau^2} + \kappa\frac{\partial^4 w}{\partial\xi^4} + a_1 w\frac{\partial}{\partial\tau}\left(w\frac{\partial w}{\partial\tau}\right) = 0 \tag{16}$$

where

$$\begin{aligned} &\omega_0^2 = \beta^2 \tfrac{n^2(n^2-1)^2}{12(n^2+1)}, \quad \mu = \alpha^2\beta^2 \tfrac{(n^2-1)(n^2-1+\nu)}{6(n^2+1)}; \quad \gamma = \tfrac{\alpha^2}{n^2(n^2+1)}, \\ &\kappa = \tfrac{\alpha^4(12+n^4\beta^2)}{12n^2(n^2+1)} \simeq \tfrac{\alpha^4}{n^2(n^2+1)}; \quad a_1 = \tfrac{(n^2-1)^4}{2n^2(n^2+1)} \end{aligned} \tag{17}$$

and only the main order terms are taken into account (see [2] for details).

The frequency gap ω_0 is small because the effective thickness is slight. We introduce the dimensionless time, which is scaled by the gap frequency ω_0: $\tau_0 = \omega_0\tau$.

The frequency spectrum in the case of simply supported edges can be written as follows:

$$\omega^2 = \tfrac{\omega_0^2+\mu\ \pi^2k^2+\kappa\pi^4k^4}{1+\gamma\pi^2k^2}, \tag{18}$$

where k is a longitudinal wave number.

Introducing complex variables (see below) and using the multi-scale expansion, equation (16) may be rewritten as follows:

$$i\frac{\partial\chi_0}{\partial\tau_2} - \frac{\mu-\omega_0^2\gamma}{2\omega_0^2}\frac{\partial^2\chi_0}{\partial\xi^2} + \frac{\kappa}{2\omega_0^2}\frac{\partial^4\chi_0}{\partial\xi^4} - \frac{a_1}{2}|\chi_0|^2\chi_0 = 0, \tag{19}$$

where the main order value χ_0 relates to the complex function $\psi = \chi_0 \exp(-i\tau_0)$. Equation (19) admits the plane-wave solution

$$\chi_0 = A\exp(-i(\omega\tau_2 - k\xi)). \tag{20}$$

where A is the amplitude. Solution (20) corresponds to the nonlinear normal mode with dispersion ratio

$$\omega = \frac{(\mu-\omega_0^2\gamma)k^2 + \kappa k^4}{2\omega_0^2} - \frac{a_1}{2}A^2, \tag{21}$$

As it can be seen, this dispersion relation is in accordance with the relation (18). The nonlinear equation (19) can be used for the analysis of the interaction of NNMs. Considering the sum of the resonant NNMs with wave numbers k_1 and k_2:

$$\chi_0 = \chi_{01}(\tau_2)\sin(\pi k_1\xi) + \chi_{02}(\tau_2)\sin(\pi k_2\xi) \tag{22}$$

we can obtain equations for the complex amplitudes χ_{01} and χ_{02}:

$$\begin{aligned} &i\tfrac{\partial\chi_{01}}{\partial\tau_2} + \delta\omega_1\chi_{01} - \tfrac{3a_1}{8}(|\chi_{01}|^2\chi_{01} + 4|\chi_{02}|^2\chi_{01} + 2\chi_{02}^2\chi_{01}^*) = 0 \\ &i\tfrac{\partial\chi_{02}}{\partial\tau_2} + \delta\omega_2\chi_{02} - \tfrac{3a_1}{8}(|\chi_{02}|^2\chi_{02} + 4|\chi_{01}|^2\chi_{02} + 2\chi_{01}^2\chi_{02}^*) = 0, \end{aligned} \tag{23}$$

where $\delta\omega_i$ are the intervals between the modal frequencies.

Equations (23) have two integrals of motion:

$$H = \delta\omega_1|\chi_{01}|^2 + \delta\omega_2|\chi_{02}|^2 - \frac{3a_1}{16}\left(|\chi_{01}|^4 + |\chi_{02}|^4\right) - \frac{a_1}{8}\left(4|\chi_{01}|^2|\chi_{02}|^2 + \left(\chi_{02}^{*2}\chi_{01}^2 + \chi_{01}^{*2}\chi_{02}^2\right)\right) \tag{24}$$

$$X = |\chi_{01}|^2 + |\chi_{02}|^2, \tag{25}$$

The solutions of equations (23) describe the evolution of the initial excitation in terms of the modes' envelopes. The detailed analysis of the Hamiltonian (24) (see [2]) for different values of the parameter X shows that, similarly to the RBM energy exchange, a slow migration of energy along the CNT occurs if the occupation number X is small enough. However, there is a critical value of X, when the energy of the CFM oscillations turns out to be captured in the initially excited region of the CNT. The evolution of the energy migration with the increase of X is shown in the fig. 4(a-c).

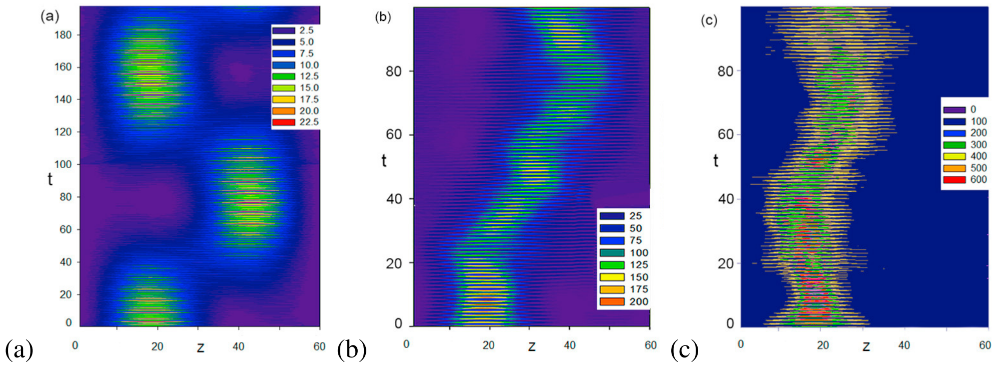

Fig. 3. (Color online) Distribution of the energy of circumferential oscillations along the CNT axis dirung the MD simulation of (20,0) CNT with aspect ratio $1/\alpha = 20$. (a) $X = 0.1X_{loc}$, (b) $X = 0.995X_{loc}$, (c) $X = 1.25X_{loc}$. The energy is measured in K, and the time - in the periods of the gap mode.

5. Conclusions

To sum up, we emphasize that the phenomenon of partial or full energy exchange is specific to the resonating nonlinear normal modes [1,2,5–8]. However, the result of intermodal interaction is determined by the relationships between the parameters of nonlinearity and the difference between frequencies, as well as by the type of nonlinear terms. The comparison of the RBM and CFM oscillations shows that in spite of the fact that both types of vibrations are optical and nonlinear resonance occurs, the distinction in the nonlinear terms leads to a distinction in the processes of energy exchange and localization.

Acknowledgments

Two of the authors (VVS and LIM) would like to thank the Russian Science Foundation (grant 16-13-10302) for the financial support of this work.

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