Energy localization in carbon nanotubes

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Abstract

In this paper, the energy localization phenomena in low-frequency nonlinear oscillations of single-walled carbon nanotubes (SWNTs) are analysed. The SWNTs dynamics is studied in the framework of the Sanders-Koiter shell theory. Simply supported and free boundary conditions are considered. The effect of the aspect ratio on the analytical and numerical values of the localization threshold is investigated in the nonlinear formulation.

1. Introduction

Carbon nanotubes (CNTs) are used as ultrahigh frequency nano-mechanical resonators in a large number of nano-electro-mechanical devices such as sensors, oscillators, charge detectors and field emission devices. The reduction of the size and the increment of the stiffness of a resonator increase its resonant frequencies and reduce its energy consumption, improving therefore its sensitivity.

The stationary or nonstationary dynamics of CNTs can be treated in terms of linear or nonlinear normal modes; in the presence of non-stationary resonance, one assists to energy transfer phenomena and formation of wave packets, having a time evolution strongly related to the spectral properties. In the nonlinear systems, the wave dispersive spreading can be compensated by the nonlinearity. As a result, a soliton mechanism of energy transfer in the quasi-one-dimensional nonlinear lattices arises.

In the present paper, the energy exchange and transition to energy capture in some part of the CNT is analysed and explained within the Limiting Phase Trajectory theory [1]. Two different approaches are used: 1) a numerical model based on the Sanders-Koiter shell theory, solved semi-analytically through a double mixed series expansion for the displacement fields; 2) an analytical model based on a reduced form of the shell theory assuming small circumferential and tangential shear deformations.

Theory

The numerical approach is based on the Sanders-Koiter shell theory, the strain and kinetic energies are written as [2]:

$$\tilde{E}=\frac{1}{2}\frac{1}{(1-\nu^2)}\left[\int_0^1\int_0^{2\pi}\left(\tilde{\varepsilon}_{x,0}^2+\tilde{\varepsilon}_{\theta,0}^2+2\nu\tilde{\varepsilon}_{x,0}\tilde{\varepsilon}_{\theta,0}+\frac{(1-\nu)}{2}\tilde{\gamma}_{x\theta,0}^2\right)d\eta d\theta+\frac{\beta^2}{12}\int_0^1\int_0^{2\pi}\left(\tilde{k}_x^2+\tilde{k}_\theta^2+2\nu\tilde{k}_x\tilde{k}_\theta+\frac{(1-\nu)}{2}\tilde{k}_{x\theta}^2\right)d\eta d\theta\right] \quad 1)$$

$$\tilde{T} = \frac{1}{2}\gamma \int_0^1 \int_0^{2\pi} (\tilde{u}'^2 + \tilde{v}'^2 + \tilde{w}'^2)\, d\eta\, d\theta \qquad \gamma = \rho R^2 \omega_0^2 / E \tag{2}$$

The displacement fields are expanded as follows:

$$\tilde{u}(\eta,\theta,\tau) = \sum_{j=1}^{N_u}\sum_{n=1}^{N} \tilde{U}^{(j,n)}(\eta,\theta)\tilde{f}_{u,j,n}(\tau)\ \tilde{v}(\eta,\theta,\tau) = \sum_{j=1}^{N_v}\sum_{n=1}^{N} \tilde{V}^{(j,n)}(\eta,\theta)\tilde{f}_{v,j,n}(\tau)\ \tilde{w}(\eta,\theta,\tau) = \sum_{j=1}^{N_w}\sum_{n=1}^{N} \tilde{W}^{(j,n)}(\eta,\theta)\tilde{f}_{w,j,n}(\tau) \tag{3}$$

where the approximate eigenfunctions are obtained through the Rayleigh-Ritz procedure explained in Ref. [2]. The resulting dynamical system is obtained by means of the Lagrange equations which are solved numerically.

It is to note that the present model does not include additional terms in partial differential equations (e.g., non-local moment, Eringen's relation) which allow to consider the "size effects". The reason is that, for the present analysis, focused on low-frequency and long SWNTs, these effects are marginal. Comparisons with Molecular Dynamics simulations confirm that our assumptions are acceptable [3].

An alternative approach is based on a reduced form of the Sanders-Koiter linear elastic shell theory developed in [2] and extended to the nonlinear field. Since low-frequency vibrations of SWNTs are considered in this work, then the elastic strain energy is predominantly due to bending, torsion and longitudinal tensions, and therefore we can neglect the circumferential and tangential shear strains of the middle surface. Due to these assumptions, the longitudinal and circumferential displacements can be expressed via the radial one. Details are omitted for the sake of brevity.

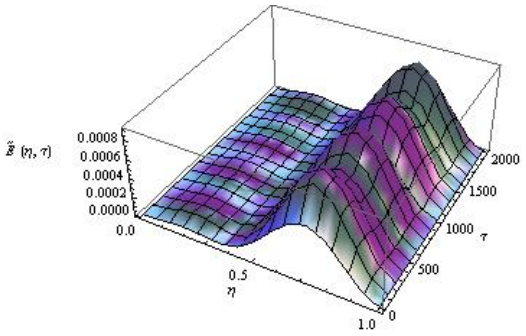

Figure 1. Energy localization: simply supported

Numerical Results

In Figure 1, the total energy distribution over the CNT surface is represented (simply supported edges). When the total energy of vibration is sufficiently high, then the combination of the two modes (1,2) and (2,2) results in a strong localization of the total energy distribution. This is a nonlinear phenomenon as the localization disappears when the vibration energy is low enough (or the system is linearized).

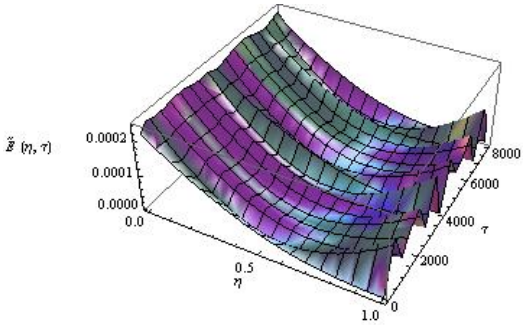

Figure 2. Energy localization: free-free

The same phenomenon appears in the case of a free-free SWNT (modes (0,2) and (1,2)), Figure 2. Also in this case the localization takes place when the vibration energy is sufficiently high.

Figure 3 clarifies that an energy threshold exists for the onset of localization. Different energy levels are needed for simply supported or free-free SWNTs, the behaviour is similar when the aspect ratio is varied, i.e., an asymptotic energy level is found for long SWNTs.

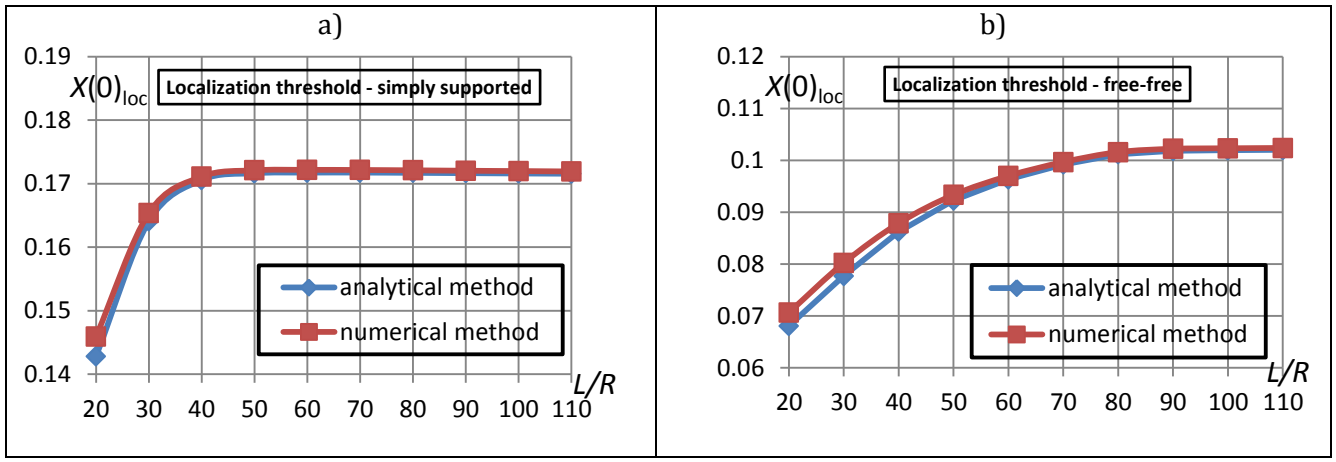

Figure 3. Localization threshold: a) simply support; b) free-free boundary conditions

Conclusions

In this paper, the low-frequency oscillations and energy localization of SWNTs are analysed within the framework of the Sanders-Koiter shell theory. The circumferential flexure modes are considered. Simply supported and free boundary conditions are studied. Two different approaches are compared, based on numerical and analytical models. For the free boundary conditions, the energy localization threshold value at the horizontal asymptote is lower than the corresponding value for the simply supported boundary conditions, since in this particular case the uniform vibrational mode with zero longitudinal half-waves loses its stability at a relatively low energy level.

Bibliography

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