Modeling and Simulations of the Nonlinear Dynamics of Carbon Nanotube Based Resonator Assuming Nonlocal Strain and Velocity Gradient Theories

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Summary. In this work, the mutual influence of the nonlocal behavior superimposed to the size effects on the dynamics of electrically actuated single walled carbon nanotube based resonator are examined. In this regards, two nonlinear models to capture the nano-structure nonlocal size effects are considered: the strain and the velocity gradients theories. A reduced-order model based on the Differential-Quadrature Method (DQM) to discretize the governing nonlinear equation of motion and acquire a discretized-parameter nonlinear model of the system is investigated. Both model results show that non-local as well size effects should not be neglected since they somehow improve the prediction of corresponding dynamic amplitudes and most importantly the critical resonant frequencies of such nano-resonators.

Introduction

Thanks to their amazing electro-mechanical features, carbon nanotubes (CNTs) and their respective compounds have shown potential applications in numerous electronic devices, energy storage, smart materials and composites, sensors and actuators and etc... Consequently, a lot of researchers and scientists worldwide [1-5] have been attracted to investigate their interesting physio-mechanical properties by introducing non-classical models. Several non-classical continuum theories have been presented and developed to pave the way for precisely extracting the size-dependent behavior of CNTs for future applications. To cite few, nonlocal theories [1] and strain gradient elasticity theory [2] are very useful to account for the nanoscale characteristics of nanostructures. In nonlocal theories, it is assumed that the stress at a specific point is a function of the strains of that point and its neighborhood as well [3]. It is demonstrated that the nonlocal theories only consider the inter-atomic long-range force [4] and the gradient elasticity theory exclusively takes into account the higher-order microstructure deformation mechanism [5]. From another point of view, the gradient elasticity theory captures the hardening behavior of nanoscale structure and, on the contrary, can only model the softening behavior of nanostructures like CNTs [4]. Therefore, in order to predict two different behaviors simultaneously and combine both possible features in nanoscale structures, it is convenient to merge two theories to bring into account two distinct properties at the same time. The key motivation behind this research work is to conduct a comprehensive study to account for the nonlocality of the stress in nanostructures incorporating the complete gradient elastic analysis of structures, that is to say, the strain and velocity gradients are included in the generalized governing equations.

Problem formulation

The investigated CNT-based resonator, Fig.1, is triggered by its lower substrate with an assumed initial gap width d. The CNT will be assumed as a cylindrical beam shape of radius $\tilde{R}$, and length L. The area moment of inertia of $I=\pi\tilde{R}^4/4$ and a resultant cross-sectional area $A=\pi\tilde{R}^2$. It also has a Young's modulus E=1 TPa and a density ρ =1.35 g/cm^3 [6].

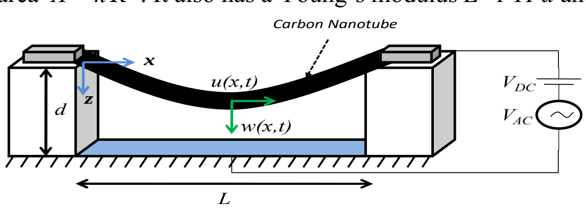

Figure 1: 3D drawing of an electrostatically actuated SWCNT based resonator.

Through considering the nonlocal effects of higher-order strain gradients $\varepsilon_{ij,k}$, in which the index k after the comma denotes the differentiation with respect to x_k, the extended Eringen's model gets the following expression for the internal potential energy as [7,8]:

$$U_0\left(\varepsilon_{ij},\varepsilon'_{ij},\alpha_0;\varepsilon_{ij,\mathrm{m}},\varepsilon'_{ij,m},\alpha_1\right)=\frac{1}{2}\varepsilon_{ij}C_{ijkl}\int_V\alpha_0\left(\left|x-x'\right|,e_0a\right)\varepsilon'_{kl}dV+\frac{l_s^2}{2}\varepsilon_{ij,m}C_{ijkl}\int_V\alpha_1\left(\left|x-x'\right|,e_1a\right)\varepsilon'_{kl,m}dV=\frac{1}{2}\int_V\left(\sigma_{ij}\varepsilon_{ij}+\sigma^{(1)}_{ijm}\varepsilon_{ij,m}\right)dV \qquad (1)$$

where e_0a and e_1a represent the influence of the inter atomic long range force and l_s stands for the strain gradient length parameter. In the framework of an Euler-Bernoulli beam theory and taking into consideration the so-called von-Karman nonlinearity, the relation for the strain-displacement of the beam (to the first order) can be written as $\varepsilon_{xx}=u_{,x}+w_{,x}{}^2/2-zw_{,xx}$. Employing the Hamilton's principle, the following normalized nonlinear governing equations of a fixed-fixed CNT resonator based on the nonlocal strain and velocity gradient theories [4]:

$$\left(1-\mu_s\frac{\partial^2}{\partial x^2}\right)\frac{\partial^4 w}{\partial x^4}+\left(1-\mu_0\frac{\partial^2}{\partial x^2}\right)\left(\frac{\partial^2 w}{\partial t^2}+\alpha_d\frac{\partial w}{\partial t}-\alpha_r\frac{\partial^4 w}{\partial x^2\partial t^2}-\alpha_s\left(\int_0^1\left(\frac{\partial w}{\partial x}\right)^2dx\right)\frac{\partial^2 w}{\partial x^2}\right)=\alpha_e\Gamma(w)+\mu_k\left(2\frac{\partial^4 w}{\partial x^2\partial t^2}-\alpha_r\frac{\partial^6 w}{\partial x^4\partial t^2}\right); \qquad (2)$$

where μ_k is the velocity gradient kinetic internal length scale and:

$$\alpha_s = \frac{Ad^2}{2I},\ \alpha_e = \frac{\pi\varepsilon_0 L^4}{EId^2},\ \alpha_r = \frac{I}{AL^2},\ \alpha_d = \tilde{c}\frac{L^4}{EI},\ \mu_0 = \left(\frac{ea}{L}\right)^2,\ \mu_s = \left(\frac{l_s}{L}\right)^2,\ \mu_k = \left(\frac{l_k}{L}\right)^2,\ \text{and}\ R = \frac{\tilde{R}}{d}, \tag{3}$$

Spatial Discretization using the Differential Quadrature Method

In order to numerically solve the nonlinear governing equation (14), we suggest to implement the Differential Quadrature Method (DQM) superimposed to the Finite-Difference Method (FDM). For the accuracy of the numerical results, the subsequent lattice distribution is assumed as $x_i = 1/2[1-\cos((i-1)\pi/(n-1))],\quad i = 1,2,\ldots n$ [9]. Therefore, for a normalized space variable x in the interval (0,1) and defining n discretization points in the space domain, the p^{th}-sequence derivative of w at point $x = x_i$ is written as $\partial^p w/\partial x^p\big|_{x=x_i} = \sum_{j=1}^{n} D_{ij}^{(p)} w_j$. The weighting coefficient matrix of the first sequence derivative is defined as $D_{ij}^{(p=1)} = \prod_{k=1,k\neq i}^{n} (x_i - x_k)/(x_i - x_j) \prod_{k=1,k\neq j}^{n} (x_j - x_k),\ i,j = 1,2,\ldots,n,\ i \neq j$

Nonlinear Dynamic Analysis: Results and Discussion

As a case study, the parameters of the studied SWCNT are considered as: d=100 nm, L=3000nm and $\tilde{R}$ =30 nm. In this work 19 discretization points is used in the DQM to get the converged results. The variation of the steady-state maximum deflection $W_{\max}$ versus the forcing AC frequency Ω is outlined in Fig. 2 for different values of the nonlocal parameter μ_0. As can be seen, when V_{DC}= 1 volt, an increase of the nonlocal parameter resulted in decreasing the maximum dynamic amplitude of the CNT. Furthermore, when considering the nonlocality effect, a softening-like behavior of the CNT is been replaced by a hardening type behavior. Figure 3 displays the frequency response of CNT for different values of the strain gradient parameter μ_s. It is evident that the maximum amplitude of the system is increased by increasing the value of DC voltage and the bandwidth expansion is increased as the DC excitation voltage increases. Figure 4 shows the frequency-response curves for three different values of velocity gradient parameter μ_k. As can be observed, the maximum dynamic deflection of the structure is considerably amplified by increasing the velocity gradient parameter and consequently the bandwidth expansion increases as the velocity gradient parameter increases.

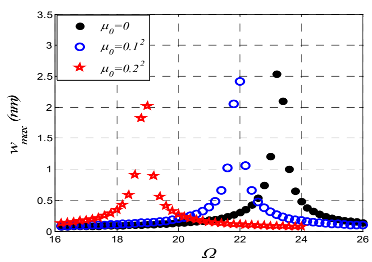

Figure 2: Dynamic response for three different nonlocal parameters for for V_{DC}= 1 *Volt*, V_{AC}= 1 *Volt*.

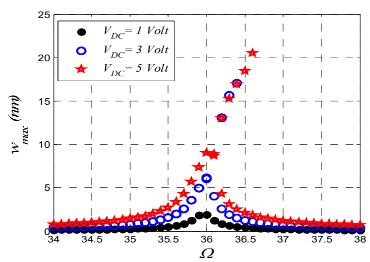

Figure 3: Dynamic response for three different values of the DC voltage for μ_s= 0.1^2.

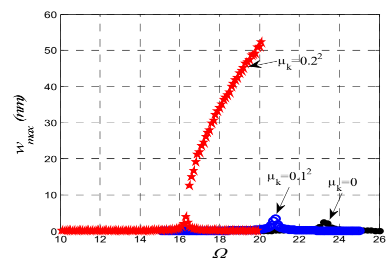

Figure 4: Dynamic response for three different velocity gradient parameters (a) VDC= 1 Volt, VAC= 1 Volt.

Conclusion

In this numerical investigation, the nonlinear dynamics of an electrically actuated doubly-clamped single-walled carbon nanotube resonator is carried out. A nonlinear Euler-Bernoulli beam model incorporating both the nonlocal and strain/velocity gradient theories is implemented. The derived nonlinear governing equation is discretized through a Differential Quadrature Method (DQM). The acquired results in this work demonstrated the fact that neglecting the nonlocal as well as the size effects imposed considerable errors in the estimation of the dynamic response of SWCNT and consequently in determining accurately its dynamical parameters such as: its resonant deflection (approx. 10-20% error) its fundamental resonant frequency (approx.15-20% error).

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