



Computational models for large amplitude nonlinear vibrations of electrostatically actuated carbon nanotube-based mass sensors



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ABSTRACT

A comprehensive multiphysics model of a cantilevered carbon nanotube (CNT) including geometric and electrostatic nonlinearities is developed. The continuous model is reduced to a finite degree of freedom system by the Galerkin discretization and solved using the harmonic balance method (HBM) coupled with the asymptotic numerical method (ANM). The influence of higher modes on the nonlinear dynamics of the considered resonator is investigated in order to retain the number of modes which will be used by the HBM+ANM procedure. Several simulations are performed for a specific CNT design in order to obtain a wide range of frequency shifts with respect to the mass and position of an added particle. This model is an intuitive way for designers to develop resonant nanosensors vibrating at large amplitudes for mass detection. Particularly, it is demonstrated that the mass and position of a particle can be determined based on the proposed model reduced to the first bending mode coupled with the analytical expressions of the linear frequency shifts for the second and third modes.

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1. Introduction

Electromechanical resonators play an important role in a variety of fields [1]. One of the most important applications is the mass detection, particularly, the detection of tiny amounts of mass [2–6]. For highly sensitive tasks, we talk about mass spectrometry. For example, mass spectrometry can provide quantitative identification of individual protein species in real time [7]. Among the most sensitive ones are sensors based on thin film [8], micron-sized cantilevers [9], the acoustic vibratory modes of crystals [10], nanocantilevers [11] and carbon nanotubes [7,12,13]. Mass spectrometers are composed by three parts: analyte ionization, analyte separation and detection [14]. These systems are widely used for several applications such as proteomics [15,16].

The micro [17]/nano [2]-electromechanical systems have large quality factors and reduced dimensions allowing to achieve femtogram ($1\text{fg} = 10^{-15}\text{g}$) [3,18], attogram ($1\text{ag} = 10^{-18}\text{g}$) [11] and zeptogram [5] ($1\text{zg} = 10^{-21}\text{g}$) resolutions. Recently, some devices can reach the mass sensitivity of the range of Dalton ($1\text{Da} = 1\text{AMU}$) [19–22]. The sensitivity of a resonant mass sensor may be established by two properties: the resonant's effective vibratory mass determined by its geometry and material properties and the stability of the frequency for long and short term governed by intrinsic and extrinsic processes [19].

Nonlinear dynamics is one of the most important properties for NEMS, allowing them to display interesting behaviors. Nonlinearities in nanoresonators can be inertial, geometric [23] or obtained by external forces [24]. A multitude of nonlinear phenomena have been observed in NEMS such as periodic attractors [25], bifurcation topology [26] and bistability [27].

Different methods have been used in order to solve the resulting non-linear equations of motion of a resonator such as the shooting method [28], time integration method [29], perturbation methods [30] and the method of non-linear normal forms [31]. In order to study the vibrational behavior of NEMS, some researches have been done using finite element-formulation [32]. For nonlinear vibrations, it is often required to calculate the periodic solutions of nonlinear differential equations. To this end, numerical methods are used. They are subdivided into two approaches: those relying on the time-domain formulation and those relying on the frequency-domain formulation. The first approach consists on transforming the original differential system into a set of algebraic equations by using an integration algorithm, and then, solving the obtained equations by continuation. The shooting method is an example of this category. The second approach is the harmonic balance method (HBM) for which the unknown variables are decomposed into truncated Fourier series. The choice between the time-domain or the frequency-domain approach depends on whether the periodic solution can be decomposed with a few Fourier components.

Cantilevered sensors are very useful for biological, chemical and physical sensors [3,33,34]. It is commonly known that the dynamic range (DR) of cantilevers is very large compared to the DR of the clamped–clamped beams (>20 times) [35]. Furthermore, the

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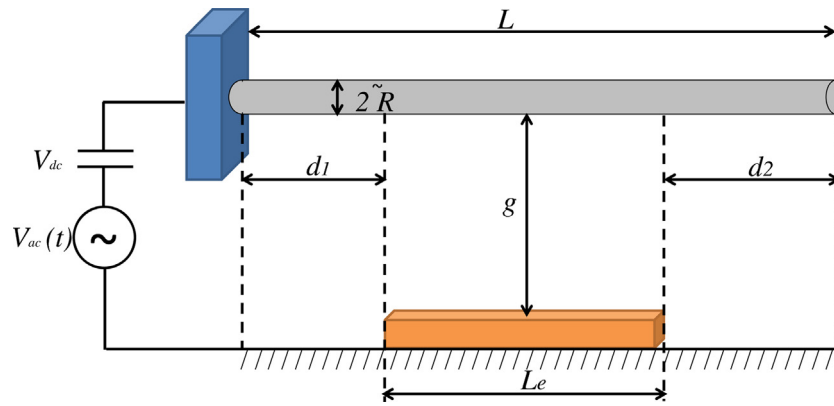


Fig. 1. Schematic of a cantilevered carbon nanotube oscillator electrostatically actuated.

miniaturization of such devices will produce nanocantilevers with higher frequencies [36] and low power consumption, which make them the most appropriate candidates for mass sensing applications.

An attached mass to a cantilever will cause the frequency shift in the fundamental mode of vibration [19,20]. The position and the mass of an added particle will change the mass response of the resonator [37]. Therefore, it is essential to provide a method allowing the simultaneous detection of the mass and position. Such method can be of a great interest for hollow cantilevers [38] in which the molecules are adsorbed on the internal surface at an unknown position. The most sensitive hollow device is the carbon nanotube, since the carbon is a material of choice for ultrasensitive resonators [39–41]. Due to the low mass of the nanotube (few attograms), a tiny amount of atoms deposited onto it represents a significant fraction of the total mass. In addition, nanotubes are mechanically ultra-rigid permitting the increase of the resonance frequency. Two major possibilities of the position of the added molecules on the resonators can be considered: the particles are added as a point mass [42] or are in a homogeneous layer covering all of the cantilever [5]. The response of the cantilever is sensitive to the variation of the position of the mass [43]. So, the particle position should be known in order to determine effectively the mass value. Several investigations were done in order to develop a technique allowing the simultaneous position and mass detection. But, such algorithms are very complicated and demand a sophisticated mathematical methods to be solved. The alternative to avoid this problem is to find relations between mass and position of the added particles and the resonant frequencies of the cantilever [44] by measuring the resonant frequencies of the beam without and with added mass for several vibrational modes.

In this paper, the nonlinear dynamics of a carbon nanotube (CNT) is investigated. To this end, a multiphysics model including the main sources of nonlinearities is developed. The mechanical nonlinearity is principally geometric while the electrostatic one is expanded in Taylor series up to the fifth order to take into account all relevant nonlinear terms for NEMS [26,45]. In order to investigate the responses of a CNT oscillator for the detection of the mass and the position of an added particle, an efficient numerical procedure has been used. The main idea is to provide numerical tools for NEMS designers in order to enhance the performances of resonant mass sensors.

Firstly, a design of an electrostatically actuated CNT is proposed and modeled. The electrode has the particularity to be placed at a specific position relatively to the nanotube in order to enlarge the NEMS dynamic range and localize a specific position of the transduction close to the fixed end of the CNT. Then, the Galerkin discretization procedure is used in order to transform the multiphysics continuum problem into a finite system of nonlinear

ordinary differential equations in time. The reduced-order model is solved numerically using the harmonic balance method coupled with the asymptotic numerical continuation technique. Based on these numerical methods, the frequency responses of the CNT for several design parameters are derived and investigated in the linear and nonlinear configurations, so that, we can retain the number of modes which gives the most accurate results.

Finally, the frequency shifts of the resonance peaks are numerically tracked on three modes for a particular CNT design and several added masses in different positions along the NEMS length. The maps of the frequency shifts are derived with respect to the mass and position of the added particle for linear and nonlinear configurations. By comparing the two cases, a hybrid analytical–numerical approach is proposed which is computationally less time consuming allowing the construction of larger frequency shift maps in order to enhance the mass detection accuracy.

2. Design and model

We consider a carbon nanotube (CNT) resonator depicted in Fig. 1. It consists of a single nanocantilever with an annular cross section initially straight, clamped at one end and free at the other end. It is actuated by an electrostatic force $v(\tilde{t}) = V_{dc} + V_{ac} \cos(\tilde{\Omega}\tilde{t})$, where V_{dc} is the dc polarization voltage, V_{ac} is the amplitude of the applied ac voltage, \tilde{t} is the time and $\tilde{\Omega}$ is the excitation frequency. The electrode is positioned at a distance d_1 from the fixed end in order to place a piezoelectric or piezoresistive transduction [46] and at a distance d_2 from the free extremity in order to enlarge the oscillator dynamic range below the upper bound limit which is the pull-in [28], since the coefficients of the bending modes are lower at $L - d_2$ in comparison with the ones at L .

The CNT is modeled as an Euler-Bernoulli beam of length L and with a quality factor Q . It has an internal radius \tilde{R}_1 , an external one \tilde{R}_2 .

2.1. Equation of motion

The equation of motion of the CNT can be written as [13]:

$$EI \partial_{\tilde{x}, \tilde{x}, \tilde{x}, \tilde{x}} \tilde{w} + \rho A \partial_{\tilde{t}, \tilde{t}} \tilde{w} + \tilde{c} \partial_{\tilde{t}} \tilde{w} = EI \partial_{\tilde{x}} (\partial_{\tilde{x}} \tilde{w} \partial_{\tilde{x}} (\partial_{\tilde{x}} \tilde{w} \partial_{\tilde{x}, \tilde{x}} \tilde{w})) + \mathcal{H}(\tilde{x}) \tilde{F} \quad (1)$$

$$\mathcal{H}(\tilde{x}) = H(\tilde{x} - d_1) - H(\tilde{x} - L + d_2)$$

where $\partial_{\tilde{x}}$ denotes the partial differentiation with respect to \tilde{x} which is the coordinate along the nanotube length L , $\partial_{\tilde{t}}$ is the partial differentiation with respect to the time \tilde{t} , $\tilde{w}(\tilde{x}, \tilde{t})$ is the in-plane bending deflection, E is the effective Young's modulus, $I = (\pi/4)(\tilde{R}_2^4 - \tilde{R}_1^4)$ is the moment of inertia of the circular cross-section, ρ is the density of the nanotube material, $A = \pi(\tilde{R}_2^2 - \tilde{R}_1^2)$

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