Design and modeling of nonlinear cantilevered carbon nanotubes electrostatically actuated for mass sensing applications

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Summary. A computational model of an electrostatically actuated cantilevered carbon nanotube (CNT) under primary resonance is developed while considering geometric and electrostatic nonlinearities. Based on the Galerkin discretization, the harmonic balance and the asymptotic numerical methods (HBM and ANM), numerical simulations are performed in order to investigate the influence of higher modes on the dynamics of the CNT. For a particular nonlinear CNT design, several frequency shifts are derived for different added masses at various positions at the resonator. It is demonstrated that a particle can be identified by the numerical simulation of the first mode coupled with the analytical formulas of the linear frequency shifts corresponding to the second and third modes.

Introduction

One of the most important applications of MEMS and NEMS devices is the mass spectrometry [1]. Several systems have been developed in order to reach ultrasensitive resolutions [2]. The cantilevered carbon nanotube (CNT) [3] is the most sensitive device for this application due to its high frequency [4], low power consumption and ultra-rigidity. In this context, a computational model of a particular design of an electrostatically actuated CNT, depicted in Figure 1 (a), including geometric and electrostatic nonlinearities [5], is developed and its application for mass detection is investigated. Since the linear dynamic range is limited [6], the principal goal is to provide numerical tools for NEMS designers, at the nonlinear regime, in order to enhance the performances of resonant mass sensors.

Design and model

The considered system is a cantilevered CNT with an annular cross section initially straight, clamped at one end and free at the other end, as depicted in Figure 1 (a). It is characterized by a quality factor Q, a length L, an internal radius $\tilde{R}_1$ and an external one $\tilde{R}_2$. It is actuated by an electrostatic force $v(\tilde{t}) = V_{dc} + V_{ac}\cos(\tilde{\Omega}\tilde{t})$, where V_{dc} the dc polarization voltage, V_{ac} the amplitude of the applied ac voltage, $\tilde{\Omega}$ the excitation frequency and $\tilde{t}$ the time. For mass sensing, a particle of mass M is placed at a distance x_M from the clamped end of the CNT. The equation of motion describing the transverse displacement of the CNT is transformed into a set of coupled nonlinear ordinary differential equations using the Galerkin discretization technique. Then, the resulting reduced order model is solved numerically by the HBM coupled with the ANM [7].

Numerical simulations

In order to investigate the impact of the number of modes on the dynamic response of the CNT without added particle, we plot numerically the frequency responses of the three first modes of the CNT for several designs. Figures 2 (a) and (b) display the frequency responses corresponding to the first mode W_{max-1} when using one, two and three modes respectively for softening and hardening behaviors. We notice slight differences when using a single or several modes [8, 9]. Consequently, a single mode is sufficient to describe accurately the dynamical behavior of the CNT. Yet, one can not solve the mass detection problem by only using one mode for two reasons. Firstly, an added particle is identified by the two unknowns the mass and the position. So, at least two modes must be used to provide two equations. Secondly, for the second mode the resonator has a node approximately at $x/L = 0.8$ (Figure 1 (b)). Thus, it is impossible to obtain the mass of a particle placed at this specific position by using only two modes.

Thereafter, the three first bending modes are needed for mass sensing. Their corresponding frequency shifts δf_{i-NL} are derived between the resonance peaks of the CNT with and without an added particle for several masses at different positions, for the design having the frequency response of Figure 2 (b). Figure 3 shows the maps of the frequency shifts of the first mode for linear and nonlinear configurations with respect to the mass and position of an added particle. Remarkably, several differences can be depicted between these two maps caused by the spring hardening effect in the frequency responses of the first mode. One can not infer the location and size of a particle from a single frequency shift because different particles can admit the same value of the shift. Since the second and the third modes have linear frequency responses for the linear and nonlinear configurations, we find perfect similarities between the maps for these two cases. Hence, a hybrid analytical-numerical approach can be used to reduce the computational time and to offer a wide range of configurations of added particles permitting the enhancement of the mass detection accuracy.

Conclusions

A specific model of a carbon nanotube electrostatically actuated and including nonlinear effects represents a very efficient tool for ultrasensitive mass detection. The mass and position of an added particle can be determined based on a hybrid analytical-numerical method which is computationally less time consuming.

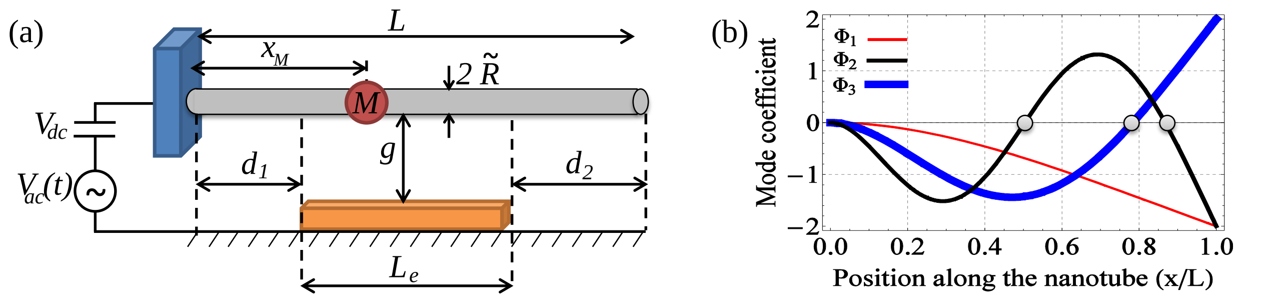

Figure 1: (a) Schematic of an electrostatically actuated cantilevered carbon nanotube with an added mass. (b) Shapes of the three first bending modes of a carbon nanotube. The gray points represent the nodes of the second and third modes.

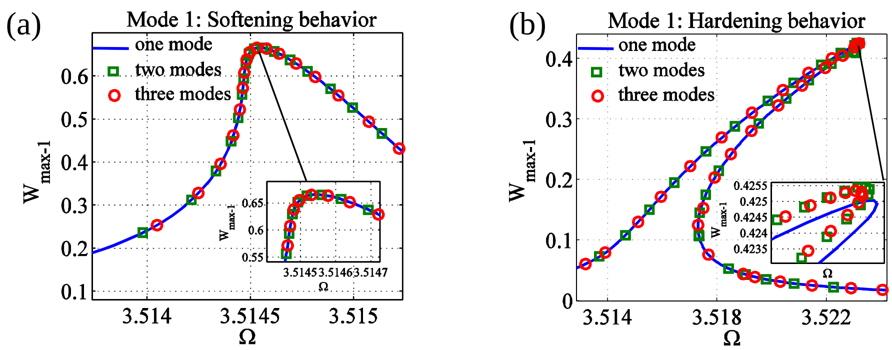

Figure 2: The frequency responses of the first mode when using one, two and three modes, where $Q = 5000$, $\frac{d_1}{L} = \frac{d_2}{L} = 0.3$ for (a) a softening behavior where $L = 20\ \mu m$, $R_1 = 180\ nm$, $R_2 = 300\ nm$, $g = 100\ nm$, $V_{ac} = 1\ V$ and $V_{dc} = 10\ V$ and (b) a hardening behavior where $L = 1\ \mu m$, $R_1 = 10\ nm$, $R_2 = 20\ nm$, $g = 100\ nm$, $V_{ac} = 2\ V$ and $V_{dc} = 15\ V$.

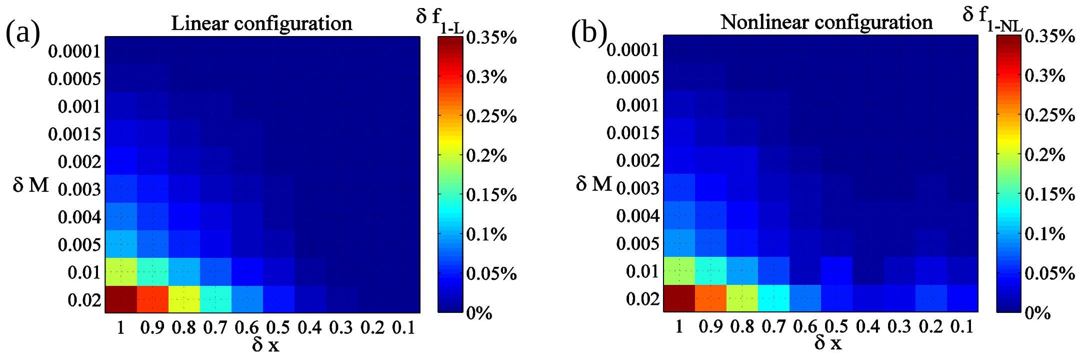

Figure 3: Frequency shifts of the first mode for (a) a linear and (b) a nonlinear configurations in the case of a hardening behavior with the following design parameters $L = 1\ \mu m$, $R_1 = 10\ nm$, $R_2 = 20\ nm$, $g = 100\ nm$, $V_{ac} = 2\ V$, $V_{dc} = 15\ V$, $Q = 5000$ and $\frac{d_1}{L} = \frac{d_2}{L} = 0.3$ for ten values of the position ratio $\delta_x = \frac{x_M}{L} \in [0.1, 1]$ and ten values of the mass ratio $\delta_M = \frac{M}{M_{CNT}} \in [0.01, 2](\%)$, where M_{CNT} is the mass of CNT.

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