Finite Elements in Analysis and Design 126 (2017) 39–49

Contents lists available at ScienceDirect

Finite Elements in Analysis and Design

journal homepage: www.elsevier.com/locate/finel

Geometrically nonlinear dynamic behavior on detection sensitivity of carbon nanotube-based mass sensor using finite element method☆

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ARTICLE INFO

Keywords:
Nonlinear dynamics
Finite element method (FEM)
Carbon nanotube (CNT)
CNT resonator
Mass sensor
Nonlinear oscillation

ABSTRACT

The principle of mass detection using carbon nanotube (CNT) resonators is based on the detection of the resonant frequency shift due to an attached mass. Although CNT resonators can easily show a nonlinear oscillation behavior, there is a lack of studies on the influence of the design parameters and the nonlinear dynamic behavior on the detection sensitivity of CNT-based mass sensors. In addition, most of the finite element method (FEM) analysis models that are used to predict the resonant frequency shift due to attached masses have been implemented in the linear oscillation regime. In order to enhance the sensing performance of the CNT-based mass sensor, a parametric study of the resonant frequency shift is conducted herein with respect to the attached mass, the electrostatic force, the initial tension and the CNT length, using an FEM-based nonlinear analysis model. The FE model is applied to solve the nonlinear dynamic behavior of CNT resonators using direct time integration and the solution is verified by its comparison to the corresponding analytical solution that had been validated in previous studies. The analysis results of the nonlinear dynamic behavior of the CNT resonator indicate that the CNT length plays a key role in the detection sensitivity, and the amount of electrostatic force determines the linear or nonlinear oscillation behavior of the resonator. It is shown that the detection sensitivity can be improved using the nonlinear oscillation behavior and this improvement is more effective with longer CNTs. This study's results justify the possibility and validity of FEM use for the analysis of the nonlinear behavior of CNT resonators and elucidate the relationship between the design parameters and the nonlinear behavior of the CNT-based mass sensor in enhancing the sensing performance.

1. Introduction

The carbon nanotube (CNT) has attracted worldwide interest and is being studied since its discovery in 1991. A CNT has unique and remarkable physical properties and has been extensively applied in various fields of research, such as in scanning probes, nanoelectronics, solar cells, ultracapacitors, diagnosis devices, and nanoelectromechanical systems (NEMS), etc. [1–3]. In the early stage of the CNT research, many studies were conducted to explore its physical properties using experimental methods and computer simulations based on molecular dynamics (MD) [4–6]. Subsequently, studies on nanoactuators and nanosensors had been actively carried out using CNTs [7,8]. Specifically, the CNT-based resonator has been successfully applied and has exhibited a high performance as a resonance-based sensor for many sensing applications, including metal deposition monitors, chemical reaction monitors, biomedical sensors, gas and mass detectors, etc. [5,8–12]. The principle of these detectors using CNT resonators is based on the shift of the resonant frequency due to the attached mass. Thus, the higher the fundamental resonant frequency of a CNT resonator is, the better is the exhibited sensitivity of detection. Based on this principle, the resonant behavior of the CNT resonator has been extensively explored in the literature [13–17]. It has been shown that the fundamental frequencies of the cantilevered or bridged CNT resonators could reach the level of 10 GHz–1.5 THz, depending on the nanotube diameter and length. Furthermore, as expected, the bridged nanotubes have higher fundamental frequencies than cantilevered ones [7,18]. Since the fundamental resonant frequency of the resonators is inversely proportional to the square of length, the sensing performance of the nanosensors is definitely enhanced upon reduction of the size of the resonators [7,19]. Therefore, a CNT constitutes the ultimate

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http://dx.doi.org/10.1016/j.finel.2016.12.002
Received 20 June 2015; Received in revised form 3 October 2016; Accepted 12 December 2016

material for these applications.

CNT resonator-based sensors provide a great potential in various applications that require very high-sensing performance. Particularly, a key point of mass detection is the quantitative analysis of the resonant frequency shifts due to the attached mass. Hence, various studies on the CNT-based mass sensor have been conducted to measure the mass attached on the CNT. It was first proposed that a CNT could be employed as a high-sensitivity nanobalance [20]. The CNT-based resonator also demonstrated feasibility and effectiveness as a high sensitive mass detector [8,21]. An application of a nanotube cantilever was then demonstrated, whereby the sensitivity for mass detection was less than a zeptogram (zg=10^{-21} g) at room temperature [22,23]. Experimentally, the detection of shifts in the resonant frequency of the nanotubes was used to sense and determine the inertial mass of atoms [24]. Based on the continuum and molecular structural mechanics approaches, single-walled carbon nanotubes (SWCNTs) were used as biosensors for detecting the mass of biological objects [18,25]. Correspondingly, the vibration signature of SWCNT was investigated to elucidate its suitability as a mass detector device using a finite element (FE) model [26]. It was reported that the vibration signature of the SWCNT-based mass sensor exhibits superharmonic and subharmonic responses with different mass levels [27].

Moreover, it was reported that because CNT-based NEMS resonators have a high-aspect ratio, a nonlinear oscillation behavior is easily exhibited owing to the large displacements. The experimental research studies showed the nonlinear dynamic behaviors elicited by the CNT oscillators [16,24] that were also studied theoretically [28–35]. An analytical solution model was proposed to analyze the nonlinear dynamic behaviors of CNT resonators using the approximation of the normal mode shape in the nonlinear equation of motion [29,36,37]. However, although it has been reported that such a nonlinear oscillation increases the resonant frequency, which may be related to the sensitivity for mass sensing, only a few research studies have been published on the nonlinear behavior of the CNT-based resonator with analytical solution methods [5,38–40]. The analytical method employs an assumed eigenmode to solve the nonlinear differential equation of a CNT resonator [29,36,37]. However, the analytical method is not appropriate as a general simulation tool for resonators with various shapes, complex geometries and boundary conditions, because the assumed eigenmode is depend to the shape and boundary condition of resonators. Especially, the nonlinear equation would not be solved when the eigenmode of CNT resonator cannot be assumed. Therefore, the analytical method with assumed eigenmode has disadvantage that it is difficult to apply to design a mass sensor using a CNT resonator with various shapes and boundary conditions.

Because the finite element method (FEM) can effortlessly handle the more complex geometries, boundary conditions and material properties, FEM has been employed to analyze a dynamic behavior of CNT resonators. However, most FEM solution models of the resonant frequency shift of CNT resonators (due to the attached mass) operating as mass sensors were implemented in the linear oscillation regime [25,27,41]. In particular, there is a lack of studies that can be utilized to the design of CNT resonators for mass sensing in the nonlinear oscillation regime, specifically, the resonant frequency shift due to design parameter (i.e. length of CNT), mass attachment and nonlinearity.

From the above discussion it is very much clear that a little work using finite element method has been reported regarding the nonlinear oscillation of CNT resonator and relationship between the design parameter of resonator and nonlinearity in order to utilize for designing the CNT-based mass sensors. Thus, the study on the nonlinear dynamic behavior and a relationship between the design parameter and nonlinearity of the CNT resonator is strongly required to design a higher performance CNT-based mass sensor. Also such study is important for future applications of CNTs.

In this study, in order to predict the shift of the resonant frequency due to the attached mass, an analysis of the dynamic behavior of the CNT resonator is implemented based on the FEM in both the linear and the nonlinear oscillation regimes. Additionally, a parametric study was conducted to elucidate the relationship between the design parameters of the CNT resonator and the nonlinear behavior that relates to the sensing performance of the CNT-based mass sensor. Because the resonant frequency shift (due to the attached mass) is related to the detection sensitivity (i.e., the sensing performance), a transient response analysis of the CNT resonators is conducted to show the resonant behavior with respect to the driving frequencies. To solve the nonlinear equation of motion for the CNT resonator owing to the consideration of the von Kármán nonlinear strain, nonlinear FEM is employed. To verify the nonlinear dynamic FE analysis model of the CNT resonators, the results of the resonant frequency are compared to the analytical solutions that had been verified in previous studies [29,36,37]. The parametric study that focuses on the resonant frequency shift is then conducted with respect to the attached mass on the CNT, the length of the CNT, the initial tension and the amount of the electrostatic force. Thus, this study constitutes fundamental research that can be utilized for the design of the CNT-based mass sensors using nonlinear oscillation behavior. This work also shows the possibility and validity of the use of FEM for the analysis of the nonlinear behavior of CNT resonators.

2. Nonlinear finite element formulation

The experimental device and the scheme proposed by Sazonova et al. are shown in Fig. 1 as an example of the nanotube oscillator for the subject of the analysis. They reported the electrical actuation and detection of the guitar-string oscillation modes of the doubly clamped nanotube oscillators and showed that the resonant frequency can be widely tuned [16]. As an example of nanomechanical resonators for the mass detection, Fig. 2 shows the experimental, doubly clamped, suspended nanotube devices with the source, drain, and gate electrodes, proposed by Chiu el al. The device detected the inertial mass of the atoms using the resonant frequency shifts of the nanotube [24].

The schematic of the doubly clamped CNT resonator used for the analysis of these mass detectors is shown in Fig. 3. The CNT resonator is actuated by the electrostatic force $p(t)$. Therefore, the equation of motion is required for calculating the resonant frequency shift due to the attached mass, m_a, with respect to the electrostatic forces. The CNT resonator assumes a continuum model with classical beam theory because the continuum mechanics method has been successfully applied to analyze the dynamic responses of individual CNTs [4,42]. A cylindrical Euler–Bernoulli beam model is considered with a radius r, an effective thickness h_{eff}, length L, Young's modulus E, density of CNT ρ_{CNT}, cross-sectional area$A$, cross-sectional moment of inertia I and the location of the attached mass on the CNT x_a.

The equation of motion for the CNT resonator can be derived using

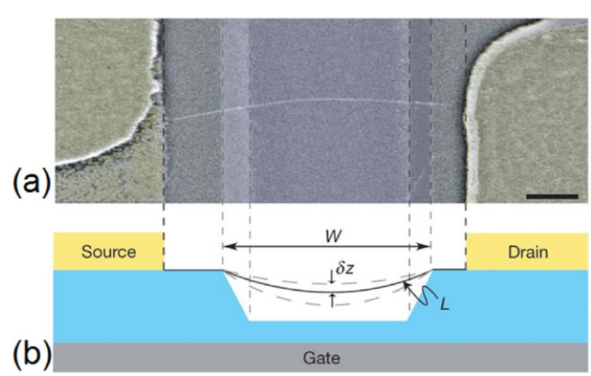

Fig. 1. (a) A scanning electron microscope (SEM) image and (b) a schematic (bottom) of the device geometry of the doubly clamped nanotube oscillators by Sazonova et al. [16].