

## NONLINEAR PERFORMANCE OF NEMS: A RESONANT MASS SPECTROMETRY

### NEMS, THIẾT BỊ CẢM BIẾN KHỐI LƯỢNG SỬ DỤNG NGUYÊN LÝ CỘNG HƯỞNG DAO ĐỘNG PHI TUYẾN

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#### TÓM TẮT

*NEMS (Nano-Electro-Mechanical Systems), hệ thiết bị cơ điện kích thước nano hoạt động dựa trên nguyên lý cộng hưởng cơ học, gần đây cho phép nhận biết các khối lượng ở thang khối lượng phân tử - cảm biến khối lượng. Các nghiên cứu trong lĩnh vực đa phần dựa trên lý thuyết dao động tuyến tính, trong khi ứng xử thực trong các hệ thiết bị này dễ dàng chi phối bởi dao động phi tuyến. Sử dụng mô hình dầm đàn hồi, bài báo nghiên cứu ảnh hưởng của dao động phi tuyến lên chức năng cảm biến khối lượng của thiết bị NEMS sử dụng ống nano carbon (CNT-based NEMS). Kết quả nghiên cứu cho thấy dao động phi tuyến làm gia tăng đáng kể độ nhạy cảm biến. Nghiên cứu làm nổi bật vai trò, tầm quan trọng của dao động phi tuyến trong công tác thiết kế, tối ưu các hệ NEMS cho mục đích cảm biến khối lượng.*

**Từ khóa:** Cơ học môi trường liên tục, NEMS, Dao động phi tuyến, Cảm biến khối lượng, Độ nhạy cảm biến.

#### ABSTRACT

*Nano-Electro-Mechanical Systems (NEMS) have recently allowed the in vitro molecular recognition. Most the detection, so far, is based on the harmonic oscillation regime, albeit nano mechanical resonators can easily reach the nonlinear vibrations. In this work, we have studied the nonlinear performance of carbon nanotube (CNT)-based NEMS for mass sensors using a continuum elastic model such as a beam model. It has been found that the nonlinear oscillation can significantly amplify the frequency shift of a CNT resonator due to mass adsorption, and consequently, the detection sensitivity of a resonator. Our study highlights the nonlinear oscillation for design and optimization of CNT-based NEMS mass spectrometry.*

**Keywords:** Continuum mechanics, NEMS, Nonlinear oscillations, Mass detection, Detection sensitivity.

#### I. INTRODUCTION

Since the discovery of carbon nanotube (CNT) [1], there are many research activities devoted to exploit their physical properties and technological applications. This is due to the fact that CNT possesses an unique structural and mechanical properties such as small size, large aspect ratio, low density, high strength, and exceptional elastic stiffness [2]; these remarkable properties make CNT to be

an ideal nanomaterial for the development of nano-electro-mechanical system (NEMS) with a wide range of applications including CNT-based scanning probes [3] nonvolatile random access memory (NRAM) [4], nano tweezers [5], nano actuators [6], and nano oscillators [7], etc. The CNT-based nano balance was first proposed by Poncharal et al [8], and recently, the feasibility of the using CNTs as nano mechanical resonators has demonstrated [9] with remarkable ability

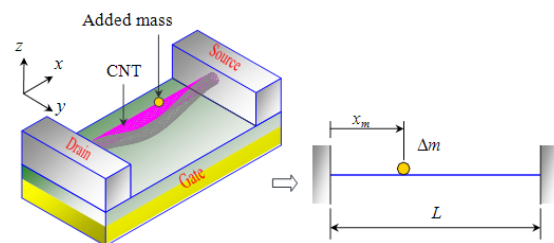
in the detection. It has been shown that, the detection sensitivity of such a nano resonator can be reached to the atomic mass resolution. This remarkable performance of nano resonators is stemmed from their ultrahigh-frequency dynamics range even up to mega- or gigahertz, which could be achieved by the scaling down of a resonator, since a resonant frequency is inversely proportional to the square of resonator length. This implies that nano resonators offer the promising future of developing of high-fidelity mass spectrometers for many sensing applications.

Most nano mechanical mass detection using NEMS resonators has been implemented in harmonic oscillation regime, albeit the NEMS resonators can easily exhibit nonlinear oscillation behavior [10]. For instance, a resonance behavior of CNT and its nano mechanical mass detection have been numerically studied by using coarse-grained model with harmonic approximation in normal mode analysis [11]. In recent studies, [12-13] the harmonic oscillation is assumed in nano mechanical detection of DNA molecule using NEMS resonator. However, in general, the actuation force can lead CNT [7] to vibrate in nonlinear oscillation. Such nonlinear oscillation behavior of CNT has been theoretically studied by continuum elastic model [14]. However, nano mechanical mass detection using nonlinear oscillation has been rarely explored, albeit nonlinear oscillation in NEMS device increases the resonant frequency related to detection sensitivity.

An effective design process of nano mechanical resonators for their specific function such as detection that requires a reliable and efficient analysis tool for understanding the dynamic behavior and sensing performance of a resonator beside experimental studies. The atomistic simulation tool such as molecular dynamics (MD) has been widely used in design of NEMS especially nano resonators [15]. However it is restricted to small length scale systems (i.e. length scale of less than

10nm) and their use become very expensive for structures of experimentally relevant sizes (i.e. hundred and/or micrometers). This limitation has led researches to consider a continuum elastic model, which is computation favorable when compared with atomistic simulations, for unveiling the vibrational characteristics of a CNT-based resonator. Remarkably, CNT has been treated as a variety of continuum models such as truss, beam, thin shell structures or a solid cylinder [16-18], where the effective elastic and structural properties (i.e., effective wall thickness  $h$ , Young's modulus  $E$ , and Poisson's ratio  $\nu$ ) of a continuum model representing CNT are determined by using atomistic simulations. Once effective properties of the nanotube are determined, a continuum elastic model can be utilized for understanding the dynamic behavior of nano resonators and their specific function such as detection. In this study, by utilizing continuum elastic model (i.e. elastic beam model), we demonstrate the role of nonlinear oscillation on the nano mechanical mass detection.

## II. THEORY & MODELING



*Figure 1. CNT-based NEMS mass spectrometry, schematic figure.*

Consider a NEMS-based resonator for mass detection as shown in Figure 1. The carbon nanotube is bridged over the trench above an electric gate. It is assumed that CNT's ends are clamped perfectly to the substrate by the van der Waals adhesion, and the vibration of the CNT is driven by electrostatic force induced from the gate. For gaining insights into the fundamental understanding the dynamic behavior of the resonator, we have assumed

that CNT can be modeled as a continuum elastic beam and that the vibration of CNT obeys the fundamental bending mode [13-14]. The equation of motion which is described the dynamic behavior of the CNT, therefore, given by

$$EI \frac{\partial^4 w(x, t)}{\partial x^4} - \left[ T_0 + \frac{EA}{2L} \int_0^L \left( \frac{\partial w(x, t)}{\partial x} \right)^2 dx \right] \frac{\partial^2 w(x, t)}{\partial x^2} + \rho(x, t) \frac{\partial^2 w(x, t)}{\partial t^2} - p(x, t) = 0 \quad (1)$$

Where  $E$ , and  $A$  are Young's modulus, cross-sectional moment of inertia, length, and cross-sectional area of CNT, respectively.  $w(x, t)$  is the CNT bending deflection as a function of coordinate  $x$  and time  $t$ .  $T_0$  is the initial mechanical tension that apply to the resonator in the axial direction and  $p(x, t)$  is the electrostatic force in the form of  $p(x, t) = p_0 f(x) \cos \Omega t$ , where  $p_0$  and  $f(x)$  are the amplitude and spatial distribution of electrostatic force respectively, and  $\Omega$  is the driving frequency. The effective mass of CNT is given by  $\rho(x, t) = \rho_{CNT} A + \Delta m(x)$ , where  $\rho_{CNT}$  is the density of CNT,  $\Delta m(x)$  is the total effective mass per unit length for adsorbed molecules onto CNT. We assume that, molecular mass adsorbed locally onto the CNT at the location of  $x = x_m$  (where  $0 < x_m < L$ ),  $\Delta m(x)$  is given by  $\Delta m(x) = \Delta m \delta(x - x_m)$ , where  $\delta$  is the Dirac delta function.

Moreover, it is assumed that molecular adsorption does not affect the bending rigidity  $EI$ , since the Young's modulus of CNT is in the order of 1TPa [16] much larger than that of biological molecules typically in the range of 1GPa [19]. It should be also recognized that the boundary conditions due to double clamping induces the geometrical nonlinear bending motion that dictated by a term of  $(EA/2L) \int_0^L [\partial w(x, t) / \partial x]^2 dx$  in Eq. (1).

For solving the equation of motion given by Eq. (1), we have employed the Galerkin's method that assumes the bending deflection

$w(x, t)$  in the form of  $w(x, t) = \phi(x) z(t)$ , where  $\phi(x)$  is the assumed deflection eigenmode. Here, we have used the deflection eigen mode of the CNT oscillator that without considering any geometric nonlinear and molecular adsorption for the assumed deflection eigen mode  $\phi(x)$  i.e  $\phi(x) = \sqrt{2/3} [1 - \cos(2\pi x/L)]$ , which satisfies the essential boundary conditions such as  $\phi(0) = \phi(L) = \phi'(0) = \phi'(L) = 0$ , where prime indicates the differentiation with respect to coordinate  $x$ . The spatial distribution of the electrostatic force in this study is assumed to be the same form with deflection eigenmode i.e.,  $f(x) \equiv \phi(x)$  The Galerkin's method apply to Eq. (1), which lead to

$$\int_0^L [Eq. (1)] \phi(x) dx = 0 \quad (2)$$

If boundary conditions are effective, Eq. (2) can be expressed as

$$\lambda \ddot{z}(t) + (\alpha + \beta T_0) z(t) + \gamma [z(t)]^3 = F_0 \cos(\Omega t) \quad (3)$$

Where

$$\lambda = \rho_{CNT} A \int_0^L \phi^2(x) dx + \Delta m \phi^2(x_m) \quad (3a)$$

$$\alpha = EI \int_0^L \left[ \frac{d^2 \phi(x)}{dx^2} \right]^2 dx \quad (3b)$$

$$\beta = \int_0^L \left[ \frac{d\phi(x)}{dx} \right]^2 dx \quad (3c)$$

$$\gamma = \frac{EA}{2L} \left[ \int_0^L \left( \frac{d\phi(x)}{dx} \right)^2 dx \right]^2 \quad (3d)$$

$$F_0 = \int_0^L p_0 [\phi(x)]^2 dx \quad (3e)$$

The specifying of the effective mechanical properties (i.e., effective thickness  $h$  and effective modulus  $E$ ) of a carbon nanotube for numerical simulation is important. There is a disagreement on values of the effective thickness  $h$  and effective modulus  $E$  of CNT in published researches up to date. However, almost researchers agree on that the effective

modulus of CNT is in the order of 1TPa and still have a debate on the effective thickness. In this study, we have used the value of effective modulus and thickness that from the Ref. [20], specifically  $E = 1030$  GPa and  $t = 0.094$  nm.

### III. RESULTS AND DISCUSSION

#### 1. Resonance behavior

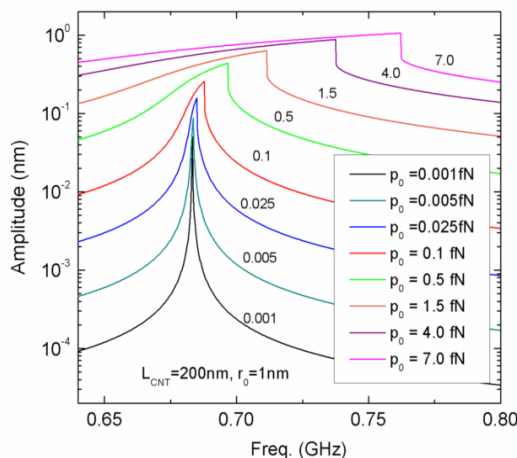
To verify our formulation, first we take into account the resonance behavior of CNT that undergoes harmonic oscillations.

**Table 1. The comparison in resonance frequency for the first mode**

$r_o/L_{CNT}$ (nm)	Present study (MHz)	Theoretical results (MHz)	Exp. results (MHz)
0.7/193	498.08	488.90	573 [21]
0.6/465	72.30	70.96	260 [21]
2.0/572	173.12	169.93	290 [21]
1.0/640	67.72	65.49	30 [21]
1.0/1750	8.92	8.76	5.1 [7]

Table 1 shows the comparisons for 6 resonators that we can find their experimental data in recent studies. The theoretical resonant frequencies in table 1 are extracted by utilizing the classical continuum mechanics theory for a linear beam with clamped ends, i.e.

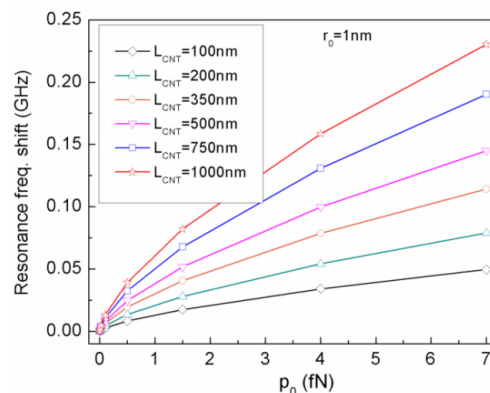
$$\omega = (4.73/L_{CNT})^2 (EI/\rho_{CNT}A)^{1/2}$$



*Figure 2. Resonance curves for CNT with its length of 200nm with respect to electrostatic forces.*

It is shown that the experimental measured resonance frequency of some CNT is higher than that from present study and the other is lower. We attribute this behavior to initial tension or slack that induces from manufacturing or the additional mass of contamination adsorbed on the CNT. The initial tension will increase the resonance frequency while the slack and contamination mass adsorbed induce decreasing in resonance frequency. Above comparisons allow us to conclude that our formulation is reasonable and can be utilized to study the dynamics behavior of the resonator that experiences linear/nonlinear oscillations as well as their response to mass adsorption.

Now, let us consider the resonance behavior of the resonator that experiences nonlinear vibrations. Figure 2 shows the resonance curves for CNT with its length of 200nm as a function of electrostatic forces. It is found that, small amount of electrostatic force (i.e.,  $p_0 \leq 25aN$ ) induces the harmonic oscillation of CNT, while large amount of electrostatic force (i.e.,  $p_0 \geq 0.1fN$ ) drives the nonlinear oscillation of CNT. The resonance frequency shifts due to electrostatic forces of resonators that possess different CNT length depicted in Figure 3. It is found that, nonlinear oscillation significant improves the resonance frequency of the resonator and that the CNT length plays a role in determine the nonlinear oscillation of a resonator.



*Figure 3. Resonance frequency shifts due to electrostatic force with respect to CNT length.*

## 2. Resonance-based mass detection

Although recent studies [11, 21] have investigated the resonant response of CNT-based resonators to mass adsorption however they confine their study to the harmonic vibrations albeit the NEMS resonators can easily exhibit nonlinear oscillations [7, 10]. It is very hard to find out studies on mass detection using nonlinear oscillations up to date except theoretical study by Buks et al., [22]. Moreover as our discussion before, nonlinear oscillations can improve the resonant frequency that may relate to detection sensitivity of resonators. It is therefore essential to study of detection behavior of resonators that experience nonlinear oscillations. To this end, we consider the locally mass adsorption onto the CNT resonator with its size of 350nm vibrates in linear (i.e.,  $p_0 \leq 25aN$ ) or nonlinear (i.e.,  $p_0 \geq 0.1fN$ ) oscillations. The resonance frequency shifts due to mass adsorption as a function of the amount of adsorbed mass are depicted in Figure 4.

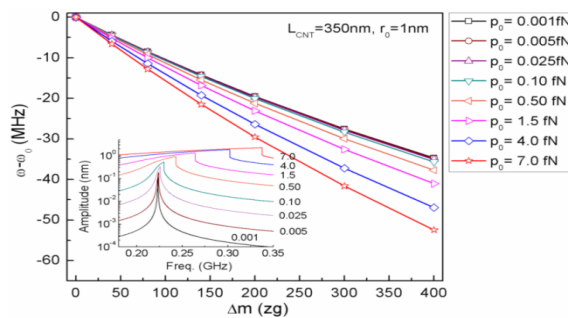


Figure 4. Resonance frequency shifts due to mass adsorption with respect to electrostatic force for resonator with its length of 350 nm.

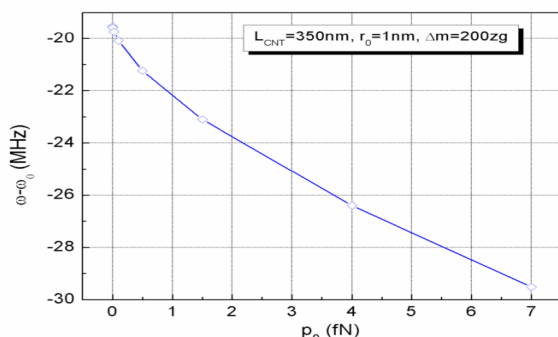


Figure 5. Resonance frequency shifts due to mass adsorption (i.e., 200zg) as a function of electrostatic force.

It is found that mass adsorption induces decreasing in resonance frequency. In linear oscillation regime the resonance frequency shift due to mass adsorption is linearly proportional to the amount of adsorbed mass regardless how much is the electrostatic force applied. This behavior is consistent with typical nano mechanical mass detection implemented in harmonic oscillation [9, 23]. However, in nonlinear vibration regime the resonance frequency shift due to mass adsorption depends not only on the amount of mass adsorbed but also the amount of electrostatic force. This indicates that electrostatic force plays a role on the detection sensitivity of a resonator that operating in nonlinear oscillation. To elucidate the role of electrostatic force on detection sensitivity of resonators, we measure the resonance frequency shifts due to mass adsorption (of 200zg) is a function of electrostatic force for the resonator with CNT length of 350nm (see Figure 5). It is interestingly shown that the detection sensitivity of the resonator is linearly enhanced with respect to the amount of electrostatic force.

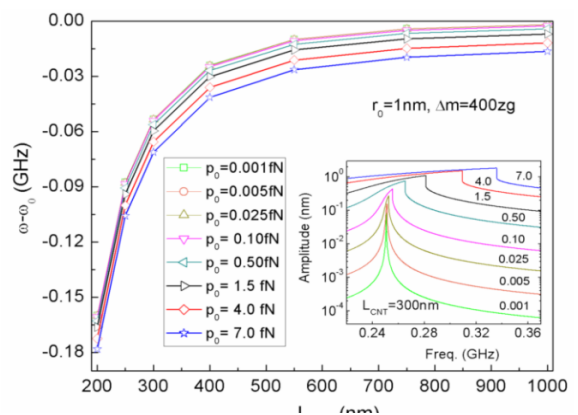


Figure 6. Resonance frequency shifts due to mass adsorption (i.e., 400zg) as a function of CNT length and electrostatic forces: Insect depicts the resonance curves for the resonator with CNT length of 300nm.

Moreover, we have studied the role of CNT length on the detection sensitivity of resonators. Indeed, Figure 6 shows the relationship between resonance frequency

shifts due to mass adsorption as a function of CNT length as well as electrostatic forces. It is clearly shown that the CNT length plays a key role in improving of detection sensitivity such that smaller length of CNT, better detection sensitivity it possess.

#### IV. CONCLUSION

In conclusion, we have demonstrated the role of nonlinear oscillation on the sensing performance of CNT resonators by considering the continuum elastic beam model. It is

shown that in harmonic vibration regime scaling down a resonator plays a dominant role in improving detection sensitivity while in nonlinear oscillation regime electrostatic force plays the vital role in enhance detection sensitivity of resonators. This implies that, nonlinear vibration is a useful route to improve the detection sensitivity for a nano mechanical resonator, and therefore it should be taken into account for design and optimization of a resonant mass spectrometry.

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