Carbon Nanotube based Mass Nano-Biosensor

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Abstract: Nano-electromechanical system based carbon nanotube is investigated as mass sensor of bio-molecules. The device in this case is modeled as carbon nanotube cantilever coupled to electronic tunneling process through such carbon nanotube. The conductance of this device is studied under the effects of magnetic field and ac-field of wide range of frequencies. Results for the conductance show periodic oscillations, which is due to photon assisted tunneling process. The resonant frequency shift and quality factor are solved numerically with dependence on the dimension of the carbon nanotube cantilever at different values of the mass of the bio-molecule. Results show both these parameters depend strongly on the length and the difference in radii of carbon nanotube. The high value of the quality factor, in the present paper, is impacted to applications of the present device to ultrafast bio-sensors and actuators. The present research can be potentially used for sensing the trace Acetone concentration in human breath, which leads to convenient, accurate and painless breath diagnosis of diabetics.
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1. Introduction:

The development of nano-electromechanical systems (NEMS) is rapidly growing due to their possible applications in various fields, such as bio-molecule detection (Arlett *et al.,* 2007), sensitive mass and displacement sensors (Yang *et al.,* 2006 and Stampfer *et al.,* 2006), energy generation (Song *et al.,* 2006), specific DNA hybridization detection (Hagan *et al.,* 2002), gas and flow sensing (Brown *et al.,* 2002), etc.

Sensors are devices that detect or sense a signal. Moreover a sensor is also a transducer, that is, it transforms one form of energy into another or responds to a physical parameter. Resonance- based sensors offer the potential of meeting the high performance requirement of many sensing applications including metal deposition monitors, chemical reaction monitors, biomedical sensors, mass detector, etc (Lu *et al.,* 1984, Benes *et al.,* 1995, Thundot *et al.,* 1997 and Hauptman *et al.,* 1998). These applications employ the characteristics of resonators in frequency shifting due to mass loading. The merit of nano-mechanical resonators is that miniaturization of their dimensions enhances the mass sensitivity of these sensors (Wenzel *et al.,* 1989). It has been reported that the detectable mass can be small as several femto grams (fg) by using micro-sized silicon or silicon nitride cantilevers (Ilic *et al.,* 2000 and Lavrik *et al.,* 2003). If the resonators are scaled down to nano-size the mass sensitivity of the resulting nanosensors can surely be enhanced. The idea of using individual carbon nanotubes (CNTs) as high sensitivity nano-balances was first proposed by the author (Poncharal *et al.,* 1999).

Since the discovery of carbon nanotube (Iijma, 1991 and Iijma, 1993) in 1991, carbon nanotubes (CNTs) have been the focus of considerable study because of their unusual strength along with excellent mechanical, electrical, thermal and magnetic properties (Dresselhaus *et al.,* 2001). CNTs are unique nano-structures which are known to have remarkable electronic and mechanical properties. These characteristics have sparked great interest in their possible uses for nano-electronic and nano-mechanical devices (Dresselhaus *et al.,* 2001, Singh *et al.,* 2007 and Sun *et al.,* 2010).In recent years; CNTs have many new applications in biomedical devices such as nano-sensors and nano-mass sensors (Arcamone *et al.,* 2006, Hoa *et al.,* 2009 and Joshi *et al.,* 2010).

The purpose of the present paper is to investigate the mass detection of bio-molecules using single walled carbon nanotube (SWCNT) cantilever coupled to two leads in order to induced electronic tunneling through this cantilever. The tunneling process is induced under the effect of magnetic field and an external ac-field of wide range of frequencies .Accordingly; we shall determine the resonant frequency shift and the quality factor of the present proposed nano-electromechanical resonator device.

2. Theoretical Treatment.

The nano-electromechanical resonator device is modeled as SWCNT cantilever connected to two metallic leads in order to induce electron

tunneling through such device. The electron tunneling through such device is studied under the effect of both magnetic field and an ac-field of different frequencies. An ac-field with frequency ω, can induce additional tunneling process when electrons exchange energy by absorbing and emitting photons of energy, $\hbar\omega$,. This kind of tunneling is known as photon –assisted tunneling (PAT) (Platero *et al.,* 2004).

Now, in order to detect the attached bio-molecule and determining its mass this can be achieved by activating the CNT to vibrate along the y-direction (Fig.1).

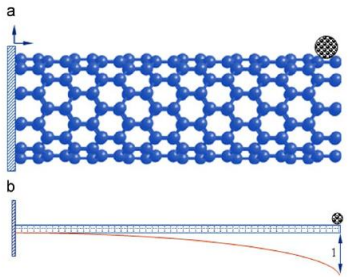

Fig.1 Sketch of CNT Cantilever

The resonant frequency shift, $\Delta\upsilon$, and the quality factor , Q, are expressed as (Lassagne *et al.,* 2009).

$$|\Delta\upsilon| = \frac{\upsilon}{2}.\frac{C_g^2.V_g^2}{k_{spring}.C_{CNT}}\left(\frac{2G}{C_{CNT}.\Gamma}-1\right) \quad (1)$$

And

$$\frac{1}{Q} = 2\pi\upsilon.\frac{C_g^2.V_g^2}{k_{spring}}.\left(\frac{2}{\Gamma.C_{CNT}}\right)^2.G \quad (2)$$

where υ is the resonant frequency of the vibrating CNT, when the bio-molecule is attached to the cantilever at one tip end (see Fig.1), C_g is the coupling gate capacitance with CNT, V_g is the gate voltage, C_{CNT} is CNT capacitance, Γ is the tunneling probability , G is the conductance of the CNT quantum device and k_{spring} is the effective spring constant of cantilever.

The effective spring constant of CNT cantilever is expressed as (Shigley, 1988 and Wu *et al.,* 2006):

$$k_{spring} = \frac{3YI}{L^3} \quad (3)$$

Where Y is Young's modulus of CNT, I its moment of inertia and L is the length of CNT cantilever.

In Eqs.(1, 2) the parameter , υ, is the resonant frequency of CNT cantilever with the attached bio-molecule on the tip of one end of CNT and is given by (Wu *et al.,* 2006 and Chowdhury *et al.,* 2009).

$$\upsilon = \frac{1}{2\pi}\sqrt{\frac{3.Y.I/L^3}{0.24.\rho.A.L+m_{bio-mol}}} \quad (4)$$

Where ρ is the density of CNT, A is its cross section area, and $m_{bio-mol}$ is the mass of the attached bio-molecule.

The conductance of the present device could be calculated by the following Landauer-Buttiker formula (Ferry *et al.,* 1997 and Bosnisk *et al.,* 2006):

$$G = \frac{4e}{h}.\sin\phi\int_{E_F}^{E_F+n\hbar\omega} dE.\Gamma_{withPhoton}(E).\left(-\frac{\partial f_{FD}}{\partial E}\right) \quad (5)$$

where $\left(-\frac{\partial f_{FD}}{\partial E}\right)$ is the first derivative of Fermi-

Dirac distribution function and it is given by:

$$\left(-\frac{\partial f_{FD}}{\partial E}\right) = (4k_BT)^{-1}.cosh^{-2}\left(\frac{E-E_F+n\hbar\omega}{2k_BT}\right) \quad (6)$$

Where k_B is Boltzman constant, T is the absolute temperature, E is the energy of the tunneled electrons, E_F is the Fermi-energy, and $\hbar\omega$ is the photon energy of the induced ac-field.

The tunneling probability ,Γ, (Eqs.1, 2, 5) has been calculated in details by the authors (Mina *et al.,* 2010 and Awadallah *et al.,* 2011) by solving the Dirac equation and applying the boundary conditions to the obtained neige functions, and its expression is given by:

$\Gamma_{withPhoton} =$

$$\sum_{n=1}^{\infty} J_n^{\,2}\left(\frac{eV_{ac}}{\hbar\omega}\right) \cdot f_{FD}\left(E - \left(\frac{C_{CNT}}{C_g}\right)eV_g - n\hbar\omega - eV_{sd}\right) \cdot \Gamma_n(E + n\hbar\omega)$$

(7)

Where J_n is the n[th] order Bessel function corresponding to the n[th] different side bands, V_{ac} is the amplitude of the induced ac-field, e is the electron charge, V_{sd} is the source-drain voltage and f_{FD} is the Fermi-Dirac distribution function. In Eq.(7), the parameter, $\Gamma_n(E + n\hbar\omega)$ is expressed as (Mina *et al.*, 2010 and Awadallah *et al.*, 2011):

$$\Gamma_n(E + n\hbar\omega) = \left|\frac{k_n}{k_n \cos(k_n L) + i\left(\frac{eV_g + eV_{sd} + \hbar eB/2m^*}{\hbar\omega}\right)\sin(k_n L)}\right|^2$$

(8)

in which k_n is given by

$$k_n^{\,2} = \left[\frac{V_b + eV_g + eV_{sd} + \hbar eB/m^*}{\hbar\omega}\right]^2 - q_n^{\,2} \qquad (9)$$

Where V_b is the barrier height at the interface between the leads and the CNT, B is the applied magnetic field , $\hbar$ is the reduced Planck's constant and m^* is the effective mass of the charge carrier.

The parameter q_n is expressed in terms of the length of CNT as follows:

$$q_n = \frac{n\pi}{L} \qquad (n=1, 2, 3, \ldots\ldots..) \qquad (10)$$

Numerical calculations will be performed to Eqs (1, 2, 5) in the next section.

3. Results and Discussion.

The present proposed CNT device based bio-molecule sensor will be analyzed numerically. This can be achieved by solving Eqs (1, 2, 5) numerically. We shall study the case of sensing of acetone molecules. It is well known that the acetone molecules exist in the breath sample of diabetic patients (Deng et al., 2004). Consequently the CNT device might be designed to target the sensing of acetone molecules and this device might be used for diabetes diagnosis.

The value of parameters in Eq.(5) for conductance (Mina *et al.*, 2010 and Awadallah *et al.*, 2011) are the following: Fermi energy, E_F, equals 0.125 eV,the effective mass of the charge carrier, m^*, equals 0.054 m_e (where m_e is the free mass of the electron),and the capacitances , C_g and C_{CNT} are 0.4nF and 0.25nF respectively.

The feature of the results for the conductance, G, are shown in Figs. 2,3 as follows:

a- Fig.2 shows the variation of the conductance G with gate voltage V_g at different values of magnetic field B. As shown from the figure that periodic oscillations of the conductance G with equal peak separation. Also, the peak height of the conductance are constant for the gate voltage, $V_g > -0.2\,V$.

b- Fig.3 shows the variation of the conductance G with the gate voltage V_g at different values of photon energy E of the induced ac-field.These values of photon energy are corresponding to photons of high frequencies, and in the range of mid-infrared region (Meyer *et al.*, 2007, Mina *et al.*, 2010 and Awadallah *et al.*, 2011).The trend of Fig.3 is similar, in quite fair, to the trend of Fig.2 .The effect of ac-field in the transport through such device might be achieved for these charge carriers with energy component E , $E \pm \hbar\omega$, $E \pm 2\hbar\omega$,…… where $\hbar\omega$ is the photon energy of the applied ac-field. These energy components are called side bands (Platero *et al.*, 2004 and Phillips *et al.*, 2008).

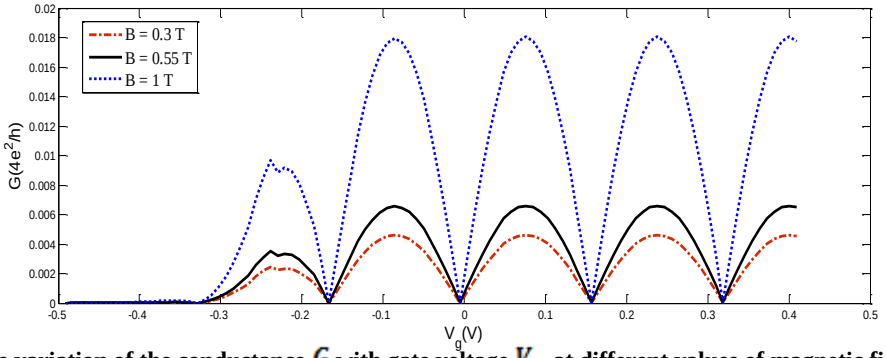

Fig.2 The variation of the conductance G with gate voltage V_g at different values of magnetic field B

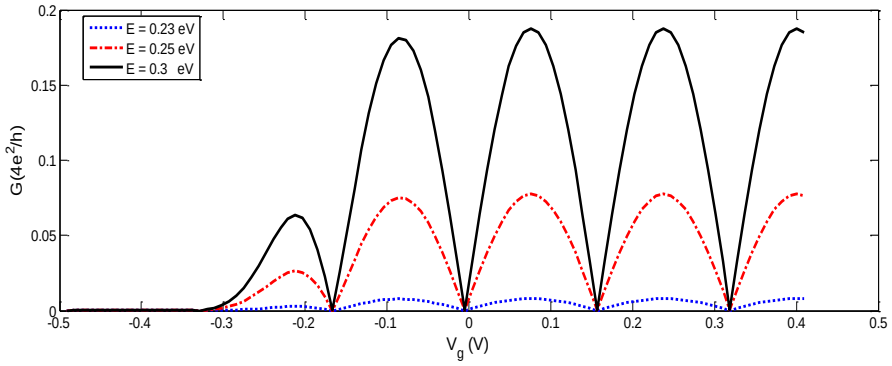

Fig.3 The variation of the conductance G with the gate voltage V_g at different values of photon energy E

The observed results might be due to transport via excited states of the CNT device. This is true that the tunneling process occurs between N-electrons excited states and the N+1 electron's ground state. This tunneling process will be enhanced by both the effect of the magnetic field and photon energy. The peak height will depend on both the quantum states and the tunneling rates involved in the tunneling process.

Now, concerning the results of the CNT based mass nano-sensor. We shall consider the acetone bio-molecule for sensing its mass. In our calculations we shall consider two cases which are :(i)Vibration of CNT cantilever, when the electron transport through CNT is off. The second case (ii) when the coupling between the electron transport and the vibration of CNT cantilever occurs.

(i)Results for the first case:

The value of Young's modulus of the CNT is equal $1.0*10^{15}$ ng/nm.S^2 and its density $\rho= 1.4*10^{-12}$ ng/nm^3 (Stampfer *et al.*, 2006, Singh *et al.*, 2007 and Chowdhury *et al.*, 2009). The resonant frequency shift $\Delta\upsilon$ is equal to the difference between resonant frequency of vibrating CNT cantilever when the bio-molecule is attached to the tip of it (Eq.4) and that resonant frequency of free CNT cantilever. i.e., $m_{bio-mol} = 0$. It is desired to calculate this resonant frequency shift $\Delta\upsilon$ with the dependence on both length ,L, of the CNT cantilever and difference in radii, ΔR, of it, So, the features of the results in this case are the following;

-Fig.(4) shows the variation of the resonant frequency shift $\Delta\upsilon$ with the length of CNT cantilever at different values of the mass of bio-molecule acetone. As shown from the figure, the resonant frequency shift $\Delta\upsilon$ decreases as the length, L, of CNT cantilever increases.

-Fig.(5) shows the cantilever of the resonant frequency shift $\Delta\upsilon$ with the difference in radii ΔR , of CNT cantilever. As shown from the figure that the resonant frequency shift $\Delta\upsilon$ increase with the increases of ΔR when $\Delta R \gtrsim 2.53$.

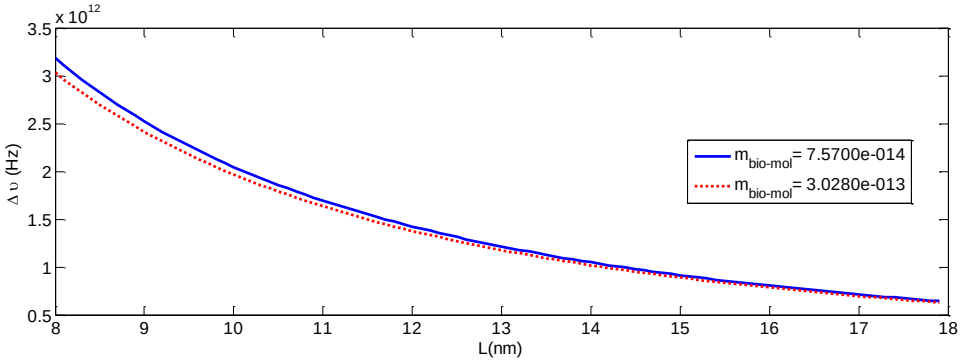

Fig.4 The variation of the resonant frequency shift $\Delta\upsilon$ with L at different values of the mass of bio-molecule acetone

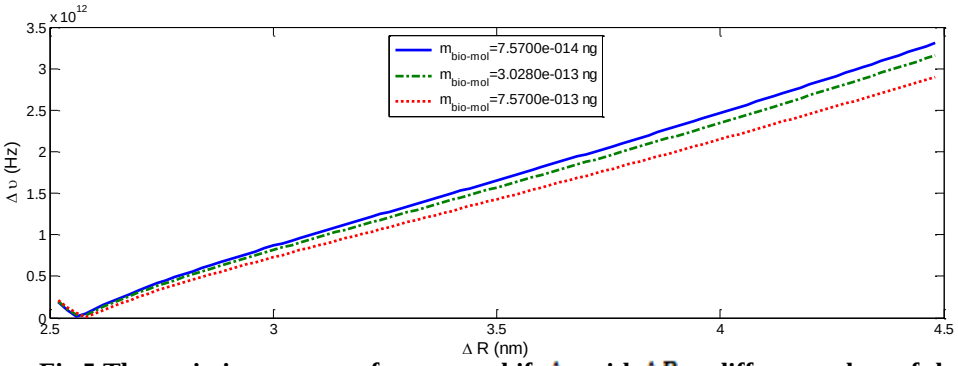

Fig.5 The variation resonant frequency shift $\Delta\upsilon$ with ΔR at different values of the mass of bio-molecule acetone

(ii)Results for the second case:

In this case the vibrating CNT cantilever as nano-electromechanical system couples to the electronic transport of this carbon nanotube. So the resonant frequency shift $\Delta\upsilon$ (Eq.1) and the quality factor , Q, (Eq.2) will be calculated. The features of the results in this case are the following:

-Fig.(6) shows the variation of the resonant frequency shift $\Delta\upsilon$ with the length L of CNT cantilever at different values of the mass of the bio-molecule acetone. As shown from the figure that $\Delta\upsilon$ increases linearly as the length, L increases. We notice from the figure that the resonant frequency shift $\Delta\upsilon$ is very small approximately $\approx 10^{-5}$ (Hz). This very small resonant frequency shift $\Delta\upsilon$ could be measured by measuring the conductance G of the CNT device. It is known that the conductance for nano-structured devices could be measured with a great precession.

-Fig. (7) Shows the variation of the resonant frequency shift $\Delta\upsilon$ with the difference in radii ΔR of CNT. As shown from the figure that $\Delta\upsilon$ decrease as ΔR increases. As in case of

Fig (6), the resonant frequency shift $\Delta\upsilon$ is very small approximately $\approx 10^{-3}$ (Hz). Also, it could be measured by measuring the conductance G.

-Fig. (8) shows the variation of the inverse of the quality factor $(1/Q)$ with the length of the CNT cantilever at different values of mass of the bio-molecule acetone. As shown from this figure that $(1/Q)$ increases as the length of CNT cantilever increases.

-Fig.(9) shows the variation of the inverse of the quality factor $(1/Q)$ with the difference in radii of the CNT ΔR at different values of mass of the bio-molecule acetone. We notice that the value of the inverse of the quality factor $(1/Q)$ decreases with the increase of ΔR.

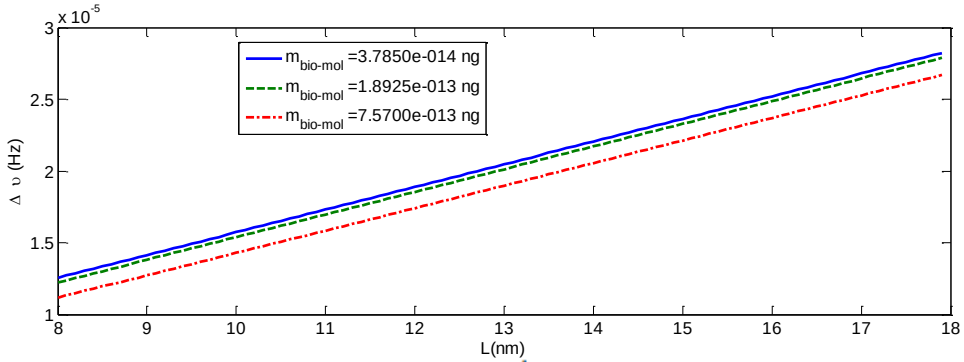

Fig.6 The variation of the resonant frequency shift $\Delta\upsilon$ with L at different values of the mass of the bio-molecule acetone

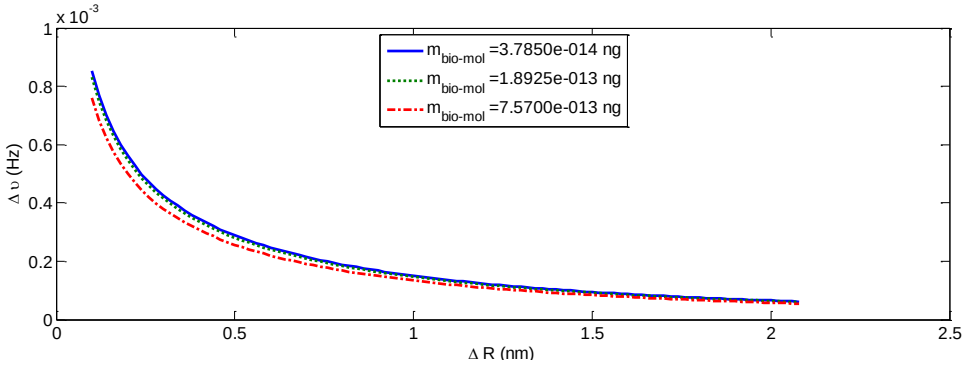

Fig.7 The variation of the resonant frequency shift Δv with ΔR at different values of the mass of bio-molecule acetone

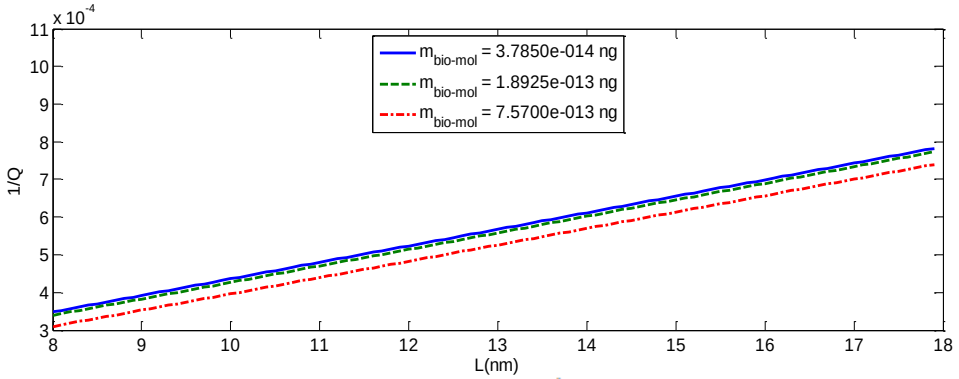

Fig.8 The variation of the inverse of the quality factor $(1/Q)$with the L at different values of mass of the bio-molecule acetone

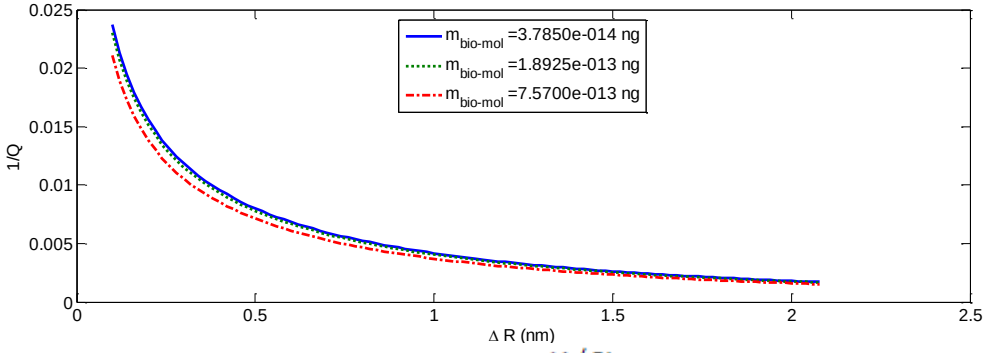

Fig.9 The variation of the inverse of the quality factor $(1/Q)$with the difference in radii of the CNT ΔR at different values of mass of the bio-molecule acetone

It must be noted that the quality factor Q (Figs 8, 9) attains a high value in the range of 10^3 - 10^5. So it is confirmed that higher quality factor means higher sensitivity and more reliable performance of the present investigated CNT based NEMS (Ekinci *et al.*, 2005). Also, these attributes makes such NEMS suitable for a multitude of technological applications such as ultrafast biosensor and actuators.

4. Conclusion.

The use of CNT based mass sensor for sensing bio-molecules has been investigated in the present paper. As shown from the present results that the resonant frequency shifts of the vibrating device could be measured by measuring the conductance of the device. So, we conclude that the present results suggest that a single walled carbon nanotube

SWCNT is a promising candidate for bio-molecular nano-sensor with very high sensitivity.

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