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Effect of the Interparticle Interactions on Adsorption-Induced Frequency Shift of Nano-beam-Based Nanoscale Mass-Sensors: A Theoretical Study

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ABSTRACT

It is well-known that the Interparticle interactions between adsorbates and surface of an adsorbent can affect the surface morphology. One of the consequences of this issue is that the resonant frequency of a nanoscale resonator can be changed due to adsorption. In this study we have chosen a cantilever-based nanoscale mass-sensor with a single nanoparticle at its tip. Using the classical continuum mechanics and the Euler-Bernoulli beam theory we have derived the governing equation of free vibration of the proposed sensor. By the assumption of physisorption, the weak van der Waals forces between the attached nanoparticle and the upper surface atoms have been taken into account. Effect of this interparticle interaction on the frequency response of the mass sensor is examined. Accordingly, the classical equation of motion has been modified by an additional term on the dynamics behavior of the sensor with a variable coefficient. It has been shown that the effect of this additional term is the same as that of an elastic foundation with variable modulus. Numerical results have shown that this additional term has significant effect on the frequency shift of a nanoscale mass-sensor in such a way that by approaching the nanoparticle towards the sensor, the frequency shift of the sensor will increase significantly. The smaller is the nanoparticle, the higher is the frequency shift.

Keywords : Nanoscale mass-sensors; Nano-beam resonators; Nano-cantilever resonators; Physisorption effects; Euler-Bernoulli beam theory.

1 INTRODUCTION

A SENSOR is a device that measures the presence or amount of substance and converts it into an interpretable signal [1]. In another view, a sensor is often defined as a device that receives and responds to a signal or stimulus. This definition is so broad that it covers almost everything from a human eye to a trigger in a pistol [2]. A mass-sensor is a special class of sensor devices in which the presence of added masses is detected. Most mass-sensors detect changes in resonant frequency of a resonator. Nowadays, miniaturization enables human beings to design and construct sensors with high enough sensitivity in micro and nano scales. There are two operation modes

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of a micro/nanoscale sensor: static mode and dynamic mode [3]. In a mass-sensor, the dynamic operation mode is used. The principle of mass detection using resonators is based on the fact that the resonant frequency is sensitive to the resonator mass, including the self-mass of the resonator and the attached mass [4]. Deposition of a nanoparticle onto a nanoscale mass-sensor leads to a change in the resonant frequency of the sensor in proportion to the amount of the mass of nanoparticle. In recent years, resonant micro/nano-electromechanical systems (MEMS/NEMS) have been the center of attention in numerous studies related to the nanoscale mass sensing. Some of these studies are devoted to nano-beam-based nanoscale mass-sensors. The reader may consult, for instant, the works of Hwang et al. [5], Bouchaala et al. [6], Mehdipour et al. [7], Mehdipour et al. [8], Kiani [9] and Kiani [10], to just name a few.
A fundamental understanding of the influence of a perturbing mass on the resonant characteristics of nanoscale sensors is a key to understanding the basis of the device's successful operation. The perturbing mass is typically one or more particles or a chemical/biological substance that adheres to or is absorbed by the sensor, thereby altering its resonant frequency [11]. Reviewing the literature reveals that some efforts have been directed toward investigation of the change of bending stiffness and the frequency shift induced by adsorbates. The reader may consult, for instant, the works of Gheshlaghi and Hasheminejad [12], Hu et al. [13], Tamayo et al. [14] and Zhang et al. [15], to just name a few. In those studies, two commonly assumptions have been made the assumption of a statistically uniform distribution of atoms or molecules adsorbed on the adsorbents and the assumption of interacting only with the nearest neighbors. By considering the later assumption, the stiffness of a micro-/nano-beam has been modified by an additional term. This additional term is written in terms of the parameters of the undeformed state (e.g., the average distance between two neighboring adsorbates in the undeformed state), hence it is a static term in this regard.

In this study, we will only consider a single attached nanoparticle. Specifically, we have chosen a cantilever-based nanoscale mass-sensor with a single nanoparticle at its tip. Using the classical continuum mechanics and the Euler-Bernoulli beam theory, we have derived the governing equation of free vibration of the proposed sensor. By the assumption of physisorption, the weak van der Waals forces between the attached nanoparticle and the upper surface atoms have been taken into account. Regarding this issue, the classical equation of motion has been modified by an additional term which has a variable coefficient. It has been shown that the effect of this additional term is the same as that of an elastic foundation with variable modulus. The effect of this additional term on the frequency response of the sensor is investigated.

2 MATHEMATICAL FORMULATIONS

From the literature, it is seen that the interaction of a single nanoparticle with a nanoscale mass-sensor has not been investigated so far. In this section, we propose a procedure to consider this issue for the first time. In what follows we consider a cantilever-based nanoscale mass-sensor with length L, width b and thickness $2h$ (see Fig.1). From the literature, one knows that in a clamped-free nanoscale mass-sensor the most mass sensitive location for mass attachment is its tip; hence, in what follows we only consider a single nanoparticle at the tip.

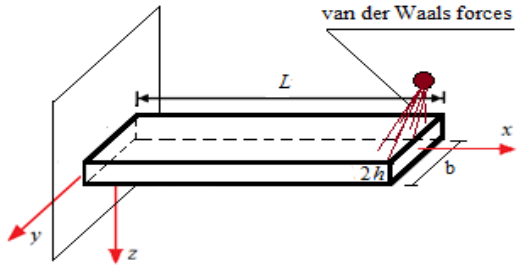

Fig.1
Schematic of the proposed sensor.

2.1 Van der Waals interaction

This subsection is mainly concerned with interparticle forces. It is well-established that between every two non-bonded and uncharged nanoparticles (e.g., two atoms or two molecules), a weak van der Waals force exists. Van der Waals forces play a central role in all phenomena involving intermolecular forces, for while they are not as strong as Coulombic or H-bonding interactions, they are always present and can be important both at small and large

separations [16]. Considering two non-bonded and uncharged nanoparticles being a distance *r* apart, the Lennard-Jones (L-J) potential may be written as:

$$V(r) = 4\varepsilon\left(\frac{\sigma^{12}}{r^{12}} - \frac{\sigma^{6}}{r^{6}}\right) \tag{1}$$

where σ is the finite distance at which the interparticle potential is zero and ε is the depth of the potential well. In this potential model, the attractive (negative) contribution varies with the inverse-sixth power of the distance and the repulsive (positive) contribution varies with the inverse-twelfth power of the distance [16].

The adsorption of nanoparticles on the surface of a nano-beam can cause it to deflect. The experimental results of Martinez et al. [17] showed that the first atomic layer on a surface plays a dominating role in the adsorption-induced deflection; hence, in this paper we assume that the interaction of the attached nanoparticle with the first atomic layer also plays a dominating role in the adsorption-induced frequency shift, and so we only consider the interaction of an attached nanoparticle with the upper surface atoms of the cantilever nanobeam.

To that end, without loss of generality, consider a nanoparticle and a differential surface element of the upper surface located at $(L, 0, h/2+d_0)$ and $(x, y, h/2+w(x,t))$ respectively; where *h* is the thickness of the nano-beam, d_0 is the vertical distance of the attached nanoparticle from the undeformed upper surface of the nano-beam and $w(x,t)$ is the flexural dynamic deflection of the nano-beam. Note that we have placed the origin of the coordinate system at the clamped end passing through the centroid with an upward *z*-axis. The pairwise interaction potential energy per unit area of a nano-resonator is written as:

$$V_{\text{int}}(x, y; X, d) = 4\varepsilon\rho_s\left(\frac{\sigma^{12}}{\left((x-L)^2+y^2+d^2\right)^6} - \frac{\sigma^{6}}{\left((x-L)^2+y^2+d^2\right)^3}\right) \tag{2}$$

where ρ_s is the number density of atoms and *d* is the instantaneous vertical distance of the attached nanoparticle from the top surface of the nano-beam which is expressed as:

$$d(x,t) = d_0 - w(x,t) \tag{3}$$

Computing the total force exerted on the attached nanoparticle by the upper surface of the nano-beam and then enforcing the equilibrium condition (i.e., $F_{total} = 0$), yields the desired equilibrium distance d_0. The total interaction energy can be calculated as given below:

$$V = \int_{-0.5b}^{0.5b}\int_{0}^{L} V_{\text{int}}\,\mathrm{d}x\,\mathrm{d}y = 4\varepsilon\rho_s\int_{0}^{L}\int_{-.5b}^{0.5b}\left(\frac{\sigma^{12}}{\left((x-L)^2+y^2+d^2\right)^6} - \frac{\sigma^{6}}{\left((x-L)^2+y^2+d^2\right)^3}\right)\mathrm{d}y\,\mathrm{d}x = \int_{0}^{L} V_y(x,d)\,\mathrm{d}x \tag{4}$$

where $V_y(x,d) = \int_{-0.5b}^{0.5b} V_{\text{int}}(x,y,d)\,\mathrm{d}y$, is the interaction potential energy per unit length of the nano-beam. By the assumption of small oscillations, the pairwise interaction energy can be approximated by the first three terms of its Taylor series with respect to the undeformed state (i.e., *w*=0) as given below:

$$V_{\text{int}}(x,y,w) = V_{\text{int}}\big|_{w=0} + \left.\frac{\partial V_{\text{int}}}{\partial w}\right|_{w=0} w + \frac{1}{2!}\left.\frac{\partial^2 V_{\text{int}}}{\partial w^2}\right|_{w=0} w^2 \tag{5}$$

One can introduce the above truncated Taylor series into Eq. (4) to obtain the total interaction potential energy as follows:

$$V(t)=\int_0^L\left[\int_y V_{\text{int}}+\left(\int_y\frac{\partial V_{\text{int}}}{\partial w}\right)w+\frac{1}{2}\left(\int_y\frac{\partial^2 V_{\text{int}}}{\partial w^2}\right)w^2\right]\mathrm{d}x=\int_0^L\left[u_0+u_1w+\frac{1}{2}u_2w^2\right]\mathrm{d}x \tag{6}$$

where the following shorthand notation has been introduced: $\int_y(\ )=\int_{-0.5b}^{0.5b}(\ )\big|_{w=0}\,\mathrm{d}y$. In what follows, we will see that only the parameter u_2 appears in the governing equation of motion.

2.2 Governing equation

2.2.1 Approach one: using Hamilton principle

In this subsection, we will derive the governing equation of the proposed nanoscale mass-sensor. According to the assumptions of the Euler-Bernoulli beam theory, the total potential energy is written as:

$$U=U_e+V=U_e+\int_0^L\left[u_0+u_1w+\frac{1}{2}u_2w^2\right]\mathrm{d}x \tag{7}$$

where U_e is the strain energy of the nano-beam. It can be simplified as:

$$U_e=\frac{1}{2}\int_0^L\iint_A\sigma_x\,\varepsilon_x\,\mathrm{d}A\,\mathrm{d}x=\frac{-1}{2}\int_0^L\left(\iint_A z\,\sigma_x\,\mathrm{d}A\right)\frac{\partial^2 w}{\partial x^2}\mathrm{d}x=\frac{-1}{2}\int_0^L M\,\frac{\partial^2 w}{\partial x^2}\mathrm{d}x \tag{8}$$

where A is the cross-section area and M is the bending moment at any cross sectional area of the nano-beam. The kinetic energy of the proposed sensor is written as:

$$T=\frac{1}{2}\int_0^L\rho A\dot{w}^2\mathrm{d}x+\frac{1}{2}m\left(\dot{w}(L,t)\right)^2 \tag{9}$$

where ρ is mass density of the nano-beam and m is the mass of the attached nanoparticle. Over-dot indicates partial differentiation with respect to time. It should be noticed that in Eq. (9), it has been assumed that the added nanoparticle is rigidly attached to the tip of the nano-beam. Now, we can use the extended Hamilton principle to obtain the governing equation and the associated boundary conditions. It can be shown that incorporating the interaction of the attached nanoparticle with the nano-beam in the formulations, alters the governing equation only. In other words, the boundary conditions will remain unchanged. The free vibration of the sensor is governed by the following partial differential equation:

$$EI\frac{\partial^4 w}{\partial x^4}+\rho A\ddot{w}+u_2w=0 \tag{10}$$

where E is the Young's modulus and I is the second moment of inertia. Note that the term u_2w is equivalent to an elastic foundation with variable modulus (remember the definition of u_2 given in Eq.(6)). The associated clamped-free boundary conditions are given below:

$$w(0,t)=\frac{\partial w(0,t)}{\partial x}=0,\frac{\partial^2 w(L,t)}{\partial x^2}=0,EI\frac{\partial^3 w(L,t)}{\partial x^3}=m\ddot{w}(L,t) \tag{11}$$

Note that the inertia of the attached nanoparticle is incorporated into the last boundary condition.

2.2.2 Approach two: modifying the classical governing equation of motion

Alternatively, one can derive the governing equation of the sensor by modifying the classical governing equation of motion as follows. One knows that the classical governing equation of free vibration of an Euler-Bernoulli beam is written as:

$$EI\frac{\partial^4 w}{\partial x^4}+\rho A\ddot{w}=q(x,t) \tag{12}$$

where $q(x,t)$ is the transverse distributed load acting on unit length of the beam for which, in the proceeding, we will derive an analytical expression. Using Eq. (1), the existed van der Waals force between two non-bonded atoms can be written as:

$$\vec{F}_{vdW}=-\frac{\partial V}{\partial r}\frac{\vec{r}}{r}=24\varepsilon\left(\frac{2\sigma^{12}}{\left((x-L)^2+y^2+(d_0-w)^2\right)^7}-\frac{\sigma^6}{\left((x-L)^2+y^2+(d_0-w)^2\right)^4}\right)((x-L)\hat{i}-y\hat{j}+(d_0-w)\hat{k}) \tag{13}$$

where $(\hat{i},\hat{j},\hat{k})$ are unit base vectors. The transverse force acting on unit length of the beam can be obtained as:

$$q(x,t)=\rho_s\int_{-0.5b}^{0.5b}(\vec{F}_{vdW}\bullet\hat{k})dy=24\varepsilon\rho_s\int_{-0.5b}^{0.5b}\left(\frac{2\sigma^{12}}{\left((x-L)^2+y^2+(d_0-w)^2\right)^7}-\frac{\sigma^6}{\left((x-L)^2+y^2+(d_0-w)^2\right)^4}\right)(d_0-w)dy \tag{14}$$

where $\bullet$ indicates the inner product of two vectors. In the case of infinitesimal deformations, one can use the truncated Taylor series to approximate the above expression with respect to the undeformed state as given below [18]:

$$q(x,t)=\int_{-0.5b}^{0.5b}\left(q_0\big|_{w=0}+\frac{\partial q_0}{\partial w}\bigg|_{w=0}w\right)dy \tag{15}$$

where, for the matters of brevity the following notation has been utilized $q_0=\rho_s\vec{F}_{vdW}.\hat{k}$. Utilizing the definition of q_0, one can simplify Eq. (14) to get the final analytical expression of the transverse force per unit length of the nano-beam as given below:

$$q(x,t)=\int_{-0.5b}^{0.5b}\left\{\begin{array}{l}24\varepsilon\rho_s\left(\dfrac{\sigma^6}{\left((x-L)^2+y^2+(d_0)^2\right)^4}-\dfrac{2\sigma^{12}}{\left((x-L)^2+y^2+(d_0)^2\right)^7}\right)\\+\left[\begin{array}{l}24\varepsilon\rho_s d_0\left(\dfrac{26\sigma^{12}}{\left((x-L)^2+y^2+(d_0)^2\right)^8}-\dfrac{7\sigma^6}{\left((x-L)^2+y^2+(d_0)^2\right)^5}\right)\\+24\varepsilon\rho_s d_0^2\left(\dfrac{8\sigma^6}{\left((x-L)^2+y^2+(d_0)^2\right)^5}-\dfrac{28\sigma^{12}}{\left((x-L)^2+y^2+(d_0)^2\right)^8}\right)\end{array}\right]w\end{array}\right\}dy \tag{16}$$

One can easily perform the above integrations by utilizing an appropriate Gauss quadrature method. In this study, we have used Gauss-Legendre quadrature rule to integrate the interparticle interaction force along the width of the nano-beam. For the purpose of free vibration analysis, in Eq. (16) we retain only those terms containing the transverse dynamics deflection; hence, Eq. (12) is rewritten as:

$$EI\frac{\partial^4 w}{\partial x^4}+\rho A\ddot{w}-\left(\sum_{k=1}^{qp}W_k\left.\frac{\partial q_0}{\partial w}\right|_{w=0,y=y_k}\right)w=0 \tag{17}$$

where qp and W_k are the total number of quadrature points and the associated weights respectively. Before presenting the solution methodology, by introducing the following non-dimensional variables in above equation, it can be rewritten as given in Eq. (19).

$$\bar{x}=\frac{2x}{L}-1,\ \bar{t}=\frac{t}{T},\bar{w}=\frac{w}{L};T=\sqrt{\frac{\rho AL^4}{EI}} \tag{18}$$

$$\frac{\partial^4\bar{w}(\bar{x})}{\partial\bar{x}^4}+\frac{1}{16}\ddot{\bar{w}}-\bar{K}(\bar{x})\bar{w}(\bar{x})=0 \tag{19}$$

where $\bar{K}(\bar{x})=\left(L^4\left(\sum_{k=1}^{qp}W_k\left.\frac{\partial q_0}{\partial w}\right|_{w=0,y=y_k}\right)\right|_{x=L/2(\bar{x}+1)}\Big/(16EI)$. In the next section, for the sake of simplicity, we will drop the overbar notation.

2.3 Free vibration analysis

In this section, we employ a pseudo spectral scheme for the purpose of free vibration analysis [19]. To do this the transverse dynamics deflection of the nano-beam is assumed to be as follows:

$$w(x,t)=W(x)e^{j\omega t}=\left(\sum_{n=1}^{N}a_nT_{n-1}(x)\right)e^{j\omega t} \tag{20}$$

where $j=\sqrt{-1}$, N is an integer number, ω is the dimensionless natural angular frequency, $a_n, n=1,2,...,N$ are unknown coefficients which will be determined in the following and $T_n(x), n=0,1,...,N-1$ are Chebyshev orthogonal polynomials. Particularly, the separation of variables technique has been employed to discretize the governing equation. Also, thanks to the completeness of Chebyshev orthogonal polynomials the spatial part of the assumed solution has been expanded in terms of these polynomials.

In the proceeding, we will use the collocation type of the proposed pseudo spectral scheme. To this end, we discretize the length of the nano-beam into *N* segments. The sampling points may be placed arbitrarily on the axis of the nano-beam. On one hand, a natural and often convenient choice for the sampling points is that of equally spaced points. On the other hand, unequally spaced sampling points may be chosen as given below:

$$x_n=-\cos\left(\frac{(n-1)\pi}{N-1}\right),n=1,2,...,N \tag{21}$$

These sampling points are called Gauss-Lobatto quadrature points which are commonly employed in the generalized differential quadrature method (e.g., [20-22]).

Now, the governing equation will be satisfied at the interior sampling points which yields *N*-4 algebraic equations. Additionally, imposition of the boundary conditions provides us with four additional equations which are necessary to complete the solution process. By introducing Eq. (20) to Eq. (19) and collocating at the interior points, one can obtain:

$$\sum_{n=1}^{N}\left(a_n\frac{d^4T_{n-1}(x_k)}{dx^4}\right)+\left(-\frac{\omega^2}{16}+K(x_k)\right)\sum_{n=1}^{N}a_nT_{n-1}(x_k)=0\ \text{for}\ k=3,4,...,N-2 \tag{22}$$

To solve this problem efficiently, we employ the concept of differentiation matrix. Considering Eq.(20), we will write the unknown coefficients in terms of the values of $W(x)$ at Gauss-Lobatto sampling points:

$$\begin{Bmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{Bmatrix} = \begin{bmatrix} T_0(x_1) & T_1(x_1) & \cdots & T_{N-1}(x_1) \\ T_0(x_2) & T_1(x_2) & \cdots & T_{N-1}(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ T_0(x_N) & T_1(x_N) & \cdots & T_{N-1}(x_N) \end{bmatrix}^{-1} \begin{Bmatrix} W(x_1) \\ W(x_2) \\ \vdots \\ W(x_N) \end{Bmatrix} = [\Gamma]\{W\} \tag{23}$$

Utilizing this concept, one can write the derivatives of the spatial mode shape functions in terms of their values at the grid points. For instant, the fourth derivative can be written as follows:

$$\begin{Bmatrix} W''''(x_1) \\ W''''(x_2) \\ \vdots \\ W''''(x_N) \end{Bmatrix} = \begin{bmatrix} T_0''''(x_1) & T_1''''(x_1) & \cdots & T_{N-1}''''(x_1) \\ T_0''''(x_2) & T_1''''(x_2) & \cdots & T_{N-1}''''(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ T_0''''(x_N) & T_1''''(x_N) & \cdots & T_{N-1}''''(x_N) \end{bmatrix} \begin{Bmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{Bmatrix} = \left[D^{(4)}\right]\{W\} \tag{24}$$

where, the prime denotes differentiation with respect to x and $\left[D^{(4)}\right]$ is the fourth-order differentiation matrix:

$$\left[D^{(4)}\right] = \begin{bmatrix} T_0''''(x_1) & T_1''''(x_1) & \cdots & T_{N-1}''''(x_1) \\ T_0''''(x_2) & T_1''''(x_2) & \cdots & T_{N-1}''''(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ T_0''''(x_N) & T_1''''(x_N) & \cdots & T_{N-1}''''(x_N) \end{bmatrix} \begin{bmatrix} T_0(x_1) & T_1(x_1) & \cdots & T_{N-1}(x_1) \\ T_0(x_2) & T_1(x_2) & \cdots & T_{N-1}(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ T_0(x_N) & T_1(x_N) & \cdots & T_{N-1}(x_N) \end{bmatrix}^{-1} \tag{25}$$

Introducing Eqs. (23) -(24) to Eq. (22) yields the following set of homogeneous equations:

$$[K_d]\{W\} = \lambda[M_d]\{W\} \tag{26}$$

where $\lambda = \omega^2$, K_d and M_d are, respectively, the stiffness and mass matrix corresponding to the interior points. These matrices are rectangular with dimension $(N-4)\times N$. Similarly, the boundary conditions are discretized as:

$$[K_b]\{W\} = \lambda[M_b]\{W\} \tag{27}$$

where K_b and M_b are the stiffness and mass matrix corresponding to the boundary conditions. These matrices are, respectively, rectangular with dimension $4\times N$ which are summarized in Appendix A. By assembling Eqs.(26)-(27) and solving the resulting eigenvalue problem, the solution process will be completed. The square roots of the eigenvalues are the natural angular frequencies of the nanoscale mass-sensor. The resonant frequencies can be obtained by dividing the natural angular frequencies by 2π .

3 NUMERICAL RESULTS

In this section, we will examine the adsorption-induced frequency shift of a nanoscale mass-sensor. To this end, we consider a graphene nanoribbon as the resonator of the proposed sensor with the following physical and geometrical properties [23]:

$$E = 1.05[TPa], \rho = 2250[kg/m^3], L = 16[nm], b = 2[nm], h = 0.34[nm], \rho_s = 3.8\times10^{19}[nm^{-2}] \tag{28}$$

In the numerical results, we have defined the resonant frequency shift denoted by Δf_n as given in the proceeding. Note that in the following definition, the interparticle interactions are incorporated into account.

$$\Delta f_n[Hz] = \frac{\omega_n - \omega_{0n}}{2\pi} \tag{29}$$

where ω_n is the nth natural angular frequency of the nano-beam with the attached nanoparticle obtained by taking into account the interparticle interactions and ω_{0n} is the nth natural angular frequency of the sensor without considering the interparticle interactions.

3.1 Results validation

Before presenting numerical results, the accuracy of the presented method of solution should be investigated. As pointed out earlier, in this paper the authors have incorporated the interactions of a single nanoparticle with the surface atoms of a nano-cantilever resonator for the first time. Considering this issue, no similar studies were found in the literature. Nevertheless, by reducing the undertaken problem to a simpler one we can obtain some reduced relations for the presented elastic nano-beam with an attached nanoparticle in this paper . More specifically, we will eliminate the effect of interaction by setting $\rho_s = 0$. Then, we compare the fundamental resonant frequencies of a cantilever single-walled carbon nanotube (SWCNT) with different added masses computed by the present study with those reported in the paper by Mehdipour et al. [4]. To this end, the following physical and geometrical properties of the SWCNT are adopted from Ref. [4]:

$$E = 32[GPa], \rho = 1330[kg/m^3], L = 5.5[\mu m], D_0 = 33[nm], D_i = 18.8[nm] \tag{30}$$

where D_0 and D_i are the outer and inner diameter of the SWCNT respectively. Table 1. depicts the fundamental resonant frequency of the SWCNT associated with different attached nanoparticles. As seen from Table 1., the fundamental resonant frequencies computed by the present study and those of Ref. [4] are almost the same. Therefore, we can conclude that the present study can be considered as the continuation study of previous works in the field of nanoscale mass-sensors.

Table 1
Comparison of fundamental resonant frequency for a clamped-free SWCNT with different attached nanoparticles.

Attached mass [*fg*]	Resonant frequency of Ref [4] [*Hz*]	Resonant frequency of the present paper [*Hz*]	% error
20	190401.8	190401.8	~0
22	181934.7	181934.7	~0
24	174505.2	174505.2	~0
26	167917.2	167917.3	~0
28	162023.2	162023.2	~0
30	156709.2	156709.2	~0
35	145419.2	145419.3	~0
40	136263.5	136263.5	~0
50	122175.3	122175.3	~0

Fig.2 shows the variation of the fundamental frequency shift with d_0. Two different nanoparticles have been moved toward the upper surface of the GNR to explore the effect of their attachments on Δf_1. As seen from this figure, approaching the nanoparticles toward the upper surface of the sensor leads to a rapid increase in the fundamental resonant frequency shift. The smaller attached nanoparticle leads to a higher fundamental resonant frequency shift.

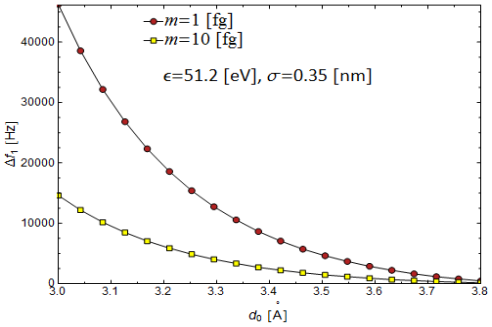

Fig.2
Variation of the fundamental resonant frequency shift $\Delta f_1[Hz]$ with the equilibrium distance d_0.

4 CONCLUSIONS

In this paper, the effect of interparticle interactions between a single nanoparticle and the surface atoms of a sensor on the frequency response of a cantilever-based nanoscale mass-sensor has been studied theoretically. By using the classical continuum mechanics and considering the assumption of physisorption, for an Euler-Bernoulli nano-beam, a new governing equation of free vibration has been established. Incorporation of interparticle interactions into account has led to a modification of the classical equation of motion by an additional term.

Chebyshev-based spectral collocation scheme has been utilized to obtain the numerical solution of the problem. To that end, the domain of the proposed sensor was discretized into finite segments. The sampling points were chosen according to the GDQM. Chebyshev orthogonal polynomials were used for spatial discretization. Imposition of the governing equation of motion on the interior sampling points altogether with satisfaction of the boundary conditions were led to a boundary value problem.

The new governing equation of motion was a fourth-order partial differential equation with a variable coefficient term. It was shown that the proposed method of solution was able to produce reliable and accurate results. Numerical results showed that the interparticle interactions have significant effect on the frequency response of a nanoscale mass-sensor. It can be concluded that in the future studies related to the nanoscale mass-sensors, the interactions of the adsorbate(s) with the sensors must be included in the mathematical formulations.

APPENDIX A

The elements of the stiffness and mass matrices corresponding to the inner sampling points are summarized below:

$$(K_d)_{ij} = D^{(4)}_{(i+2)j} - K(x_{i+2})\delta_{(i+2)j}, \qquad i = 1,2,...,N-4; j = 1,2,...,N$$
$$(M_d)_{ij} = \frac{1}{16}\delta_{(i+2)j}, \qquad i = 1,2,...,N-4; j = 1,2,...,N \tag{A.1}$$

where δ_{ij} is the Kronecker delta. Also, the elements of the stiffness and mass matrices corresponding to the boundary conditions are summarized below:

$$(K_b)_{ij} = \begin{cases} \delta_{1j}, & i = 1, j = 1,2,...,N \\ D^{(1)}_{1j}, & i = 2, j = 1,2,...,N \\ D^{(2)}_{Nj}, & i = 3, j = 1,2,...,N \\ D^{(3)}_{Nj}, & i = 4, j = 1,2,...,N \end{cases}$$
$$(M_b)_{ij} = \begin{cases} \dfrac{-M}{8\rho AL}, & i = 4, j = N \\ 0, & otherwise \end{cases} \tag{A.2}$$

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