RESEARCH PAPER

Numerical Study of a Highly- Sensitive Nanosensor for Heavy Metal Detection

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ARTICLE INFO

Article History:
Received 18 December 2025
Accepted 26 March 2026
Published 01 April 2026

Keywords:
Clean energy
Mass sensitivity
Mercury detection
Nanoelectromechanical sensor
Resonator

ABSTRACT

Heavy metals, including mercury and lead, are among the main environmental pollutants, especially in the air, stemming from industrial production processes and fossil fuel combustion. These types of industrial contaminants pose a significant risk to human health. Here, a high throughput nanosensor is introduced which detects mercury vapor through mass-loading method in real time without any label in clean energy systems. The sensor is made of a resonator that vibrates parallel to the substrate by rotary Electrostatic actuators. When voltage is applied to the actuators, the whole system oscillates at the natural frequency. Due to the fabrication method, very thin layer of gold is deposited on both sides of the resonator. In case of mercury reaction with the gold cover resonator, the mass and stiffness of the resonator change and, consequently, the output frequency shifts. These frequency changes can be measured through output current monitoring. The proposed sensor is based on Nanoelectromechanical systems technology which is compatible with chip fabrication technologies and so the required electronic components for sensing can be integrated with it. Finite element results obtained from COMSOL Multiphysics showed at the resonance frequency of 29.22 MHz, the quality factor of the sensor is as high as 730. Additionally, the sensor has a high mass sensitivity of 7 Hz/ag, indicating its potential to detect small amounts of mercury.

How to cite this article
Hadjiaghaie Vafaie R., Mehdipoor M., Zinatloo-Ajabshir S. Numerical Study of a Highly- Sensitive Nanosensor for Heavy Metal Detection, 2026; 16(2):2204-2213. DOI: 10.22052/JNS.2026.02.065

INTRODUCTION

Nanoelectromechanical systems provide the fabrication of miniature mass sensor devices that enable precise masses measurements of a gas and biological elements in the pico-gram and sub-pico-gram ranges [1-3]. Various techniques of transduction in micro and nano electromechanical systems include piezoresistive, piezoelectric, optical, capacitive, and magnetic methods, which detect and measure applied target masses as well [4-6].

Miniaturization of electromechanical sensors leads to some advantages such higher resonance frequencies, lower power requirements, fast response, high sensitivity, and high signal-to-noise (SNR) ratio [7-10].

Over the past two decades, the number of studies focusing on nanosensors and their various applications has considerably grown, which can

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provide physical and chemical characteristics of the target material. In physical measurement, physical properties such as temperature, pressure, and strain are observed, and in chemical measurement, chemical composition, reactions, and material composition are considered [11-14].

Different nanomaterials are used to enhance mercury detection, such as gold, silver, silica, and magnetic nanoparticles (AuNPs, AgNPs, SiO2NPs, and MNPs), hybrid combinations of silver and gold, quantum dots, electrochemical materials, and nanostructures based on carbon [15].

Nano-sensors based on gold nanoparticles (AuNPs) are more effective in mercury sensing, taking advantage of specific properties of gold such as stability, biocompatibility, and easy of functionalization. In these sensors, the surface plasmon resonance method can be exploited for mercury ion trace through colorimetric detection. Moreover, due to the high surface-to-volume ratio of gold nanostructures, active sites for binding with mercury ions increase, therefore, high sensitivity is achieved [16].

Silver nanoparticles (AgNPs) are one of the key components in developed sensors due to their unique optical interaction with light. This interaction is known as localized surface plasmon Resonance (LSPR), a process where sub-wavelength conductive particles contain and oscillate light waves. The resulting unique light absorption profile enables these nanoparticles to function as highly discerning and responsive indicators when exposed to target chemicals [17, 18].

Hybrid gold-silver nanoparticles (NPs) are becoming the preferred material for high-performance mercury ion detection. Their advantage stems from the combined strengths of the constituent elements: the conductive properties of Ag and the durability of Au. This bimetallic setup enhances detection limits and differentiation capability. Critically, the interface between the two noble metals offers precise control over surface chemistry, allowing for the targeted adjustment of the sensor's attraction to mercury [19, 20].

The unique characteristics of Carbon Dots (sub-10 nm carbon nanoparticles) make them ideal components for detection technology. Their distinctive optical and electronic signatures support their wide-ranging use as powerful sensor platforms. A promising area for these materials is the creation of CD-based nanosensors for mercury (Hg) analysis. These devices offer superior sensitivity and target specificity and can be finely tuned for optimal mercury affinity through surface engineering and functionalization [21, 22].

Quantum Dots (QDs), semiconductor with particles size of 2–10 nm, are chosen for their size-dependent optical and electronic adjustability. This quantum confinement effect permits the specific engineering of their band gaps, which is ideal for sensor design. Their interaction with mercury ions is characterized by clear changes

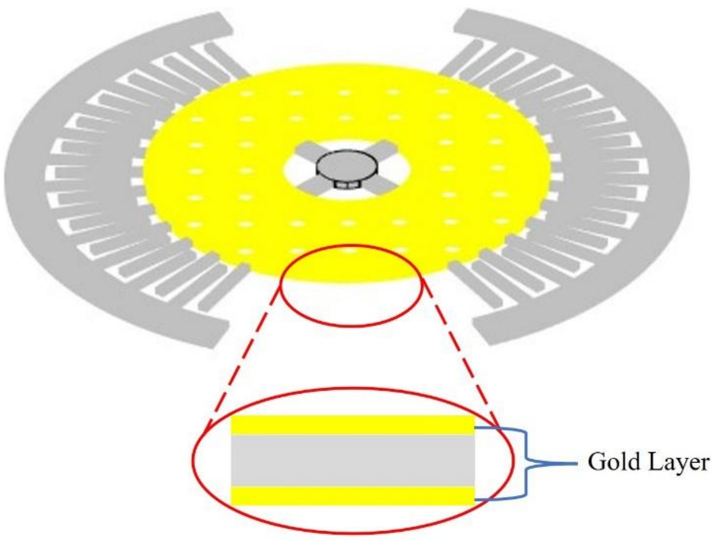

Fig. 1. Functionalized mercury sensor for clean energy application.

in fluorescence, establishing QDs as a versatile and effective platform for fast, accurate mercury detection [23, 24].

Advanced detection based on electrochemical nanosensors, offering a robust and sensitive way to find mercury. These sensors function by harnessing the electrocatalytic power of nanoscale materials, nanoparticles, or nanotubes, enabling quick and selective analysis. The key to their enhanced performance (sensitivity and specificity) lies in the precise engineering of the electrode interface and the composition of the nanostructure [25].

Silica nanoparticles are highly suitable for nanosensor construction because of their stability, biocompatibility, and flexibility. Their high surface area and tunable surface chemistry provide a powerful platform for the selective and sensitive measurement of mercury ions. To achieve this superior detection capability, silica NPs are modified with specific recognition elements (receptors), which increases their binding specificity and sensitivity toward the target metal [25, 26].

Magnetic nano-sensor (MNPs) are a popular choice for mercury sensing because of their appealing magnetic qualities, small size, and capacity for surface modification. A major advantage is that their magnetic nature simplifies the isolation of the sensing material from complex matrices. This ease of retrieval has driven extensive scientific exploration into numerous magnetic nanosensor architectures for targeted mercury detection [27, 28].

Mercury sensing can be achieved using eco-friendly nanosensors derived from versatile organic scaffolds. These sensors are generally polymer- or biomolecule-based and are chemically tailored to bind selectively with mercury ions. The organic structure facilitates biocompatibility and simplifies the tuning of performance parameters (selectivity/sensitivity). This class of nanosensors is particularly advantageous due to its modifiability and compatibility with existing detection technologies [29].

Various nanostructures for mass sensing such doubly clamped beams and cantilevers are used for different applications, with their limitations and capabilities [30-40].

The aim of this research is to design and analyze a novel mass sensor with nanoelectromechanical system that utilizes suspended gold coated resonator for detecting mercury in the picogram range. The innovative design includes the development of a configuration of resonated suspended by four springs connected to a central anchor which enable high-resolution in in-plane resonance and eliminating the additional labels for mercury trapping as shown in Fig. 1. Notably, due to miniaturized size, the mass sensor (10 × 10 µm) with gold coated surfaces is a candidate for

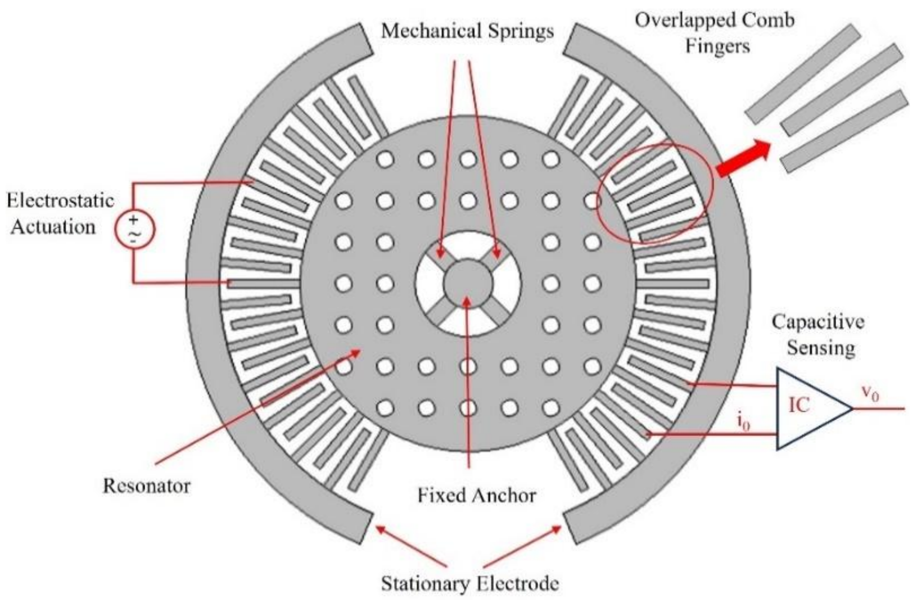

Fig. 2. Different parts of the nanosensor including a resonator, anchor, and actuating and sensing part.

various applications such as medical and health demanding [41, 42]. Furthermore, the proposed mass sensors can be integrated in a single chip with peripheral electronic for actuation and sensing parts.

This paper discusses first the design and dimension of different part of the sensor. Following this, the applied theory for damping and quality factor is expressed in details. Afterward, the dynamic response of the mass sensor is studied and discussed.

The high resonance frequency reveals that the proposed resonator is highly-sensitive enough to trace mercury vapor in clean energy purposes where good linearity of sensitivity is obtained.

MATERIALS AND METHODS

Design and Construction

The proposed nanosensor consists of a circular resonator covered by a very thin gold layer to trap mercury vapor which is connected to central anchor by four springs. Electrostatic actuator and capacitive sensing are used to drive the resonator vibrate in in-plane mode and to sense the absorbed target mass on the resonator, as shown in Fig. 2. To increase the reaction of target particles with the functionalized surface, etch holes are used in the resonator which allows the gold to be deposited under the sensor. Each set of finger has two groups of electrodes, fixed and movable, with a minimum gap between them to reach maximum momentum at low drive voltage. Using polysilicon as the body material through surface micromachining, the proposed structure can be produced without extra complexity. The total size of this nanosensor is about *10*10 μm²* with thickness of *150 nm*, and other related dimensions are shown in Fig. 3 and are listed in Table 1.

When mercury deposits on the resonator, total mass of the resonator increases therefore frequency of the sensor decrease. These frequency changes can be measured through output current between finger electrodes in sensing part. In other words, when gold reacts with mercury vapor, the capacitive value been electrodes changes and monitoring the output current results the frequency shifts.

Quality factor, Damping effect, and Sensitivity

One of the resonator specifications describing the way the sensor works is quality factor that indicates the accuracy and stability of the response in the long-term measurements. High value of quality factor indicates the sharpness

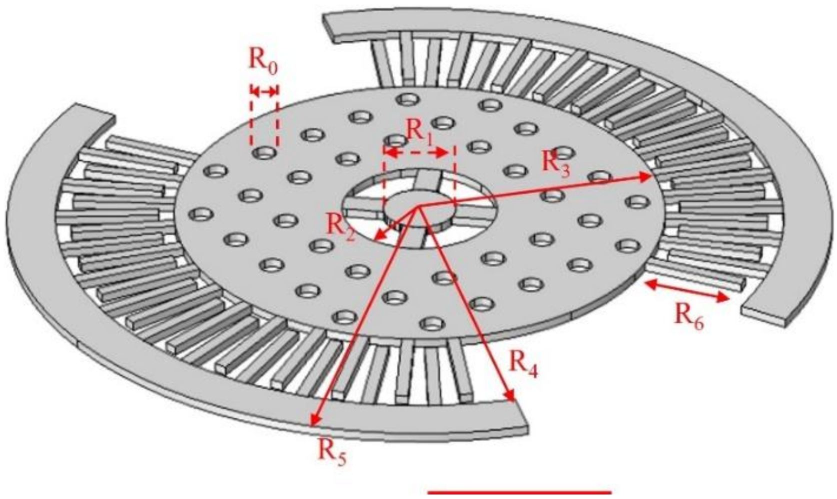

Fig. 3. Applied parameter in the design of the sensor.

Table 1. The values of different parameters shown in Fig. 3.

Parameter	R_0	R_1	R_2	R_3	R_4	R_5	R_6
Value(μm)	0.4	1.2	1.280	4.05	6	6.8	1.734

of the output signal and lower damping in a resonator. Among different damping sources, viscous damping resulting from target particles and anchor damping are considered as below:

$$\frac{1}{Q_{tot}}=\frac{1}{Q_{viscous}}+\frac{1}{Q_{anchor}} \tag{1}$$

Q_{anchor} and $Q_{viscous}$ are the quality factors of anchor and viscous damping consisting of sliding and stokes damping in the system, which are related to the damping of the gas present in the minimal distance between the sensor and the substrate, and the stokes damping due to the target particles on the reaction area, [43]. In the following, the theory behind of the two types of sliding and stokes damping are represented.

Considering the application of the introduced sensor in a gaseous environment, viscous damping is divided into two parts including damping under and on the sensor shown in Fig. 4.

Under the proposed sensor, because of high resonance frequency and very small gap between the structure and the substrate, transition flow conditions are set up (0.1< K_n<10). Thus, the damping factor follows (Eq. 2) [43]:

$$c_u=\frac{\mu A\beta_2[2+\beta_2\lambda\tanh(\beta_2 z_0)-\beta_2^2\lambda^2\tanh^2(\beta_2 z_0)]}{4\beta_2\lambda+(2+\beta_2^2\lambda^2)\tanh(\beta_2 z_0)-\beta_2\lambda\tanh^2(\beta_2 z_0)}$$

$$\beta_1=\sqrt{\frac{\omega}{2\upsilon}},\ \ \beta_2=(2j\beta_1)^{1/2} \tag{2}$$

Where, *A*,, and z_0 are angular velocity, dynamic viscosity, the sensor area, the free mean molecular path, and the gap distance, respectively.

For the stokes layer of the gas flow on the active area of the sensor, related damping coefficient is expressed as [43]:

$$c_o=\frac{\upsilon\rho A(\lambda\omega+\sqrt{2\upsilon\omega})}{\lambda^2\omega-2\upsilon} \tag{3}$$

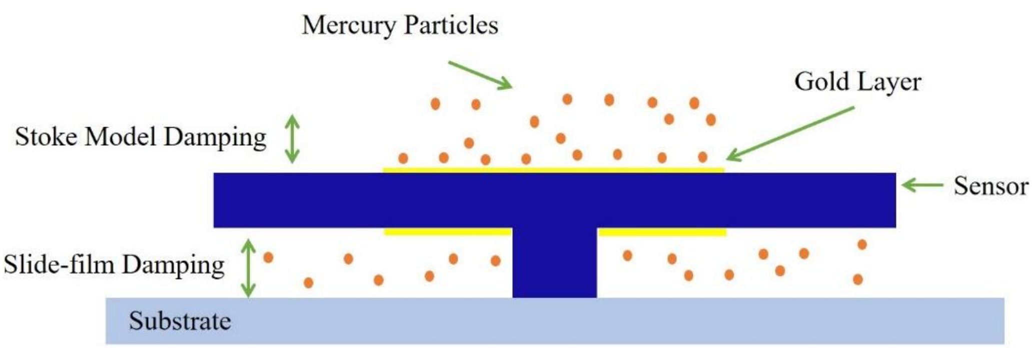

Fig. 4. Different damping sources in the proposed structure.

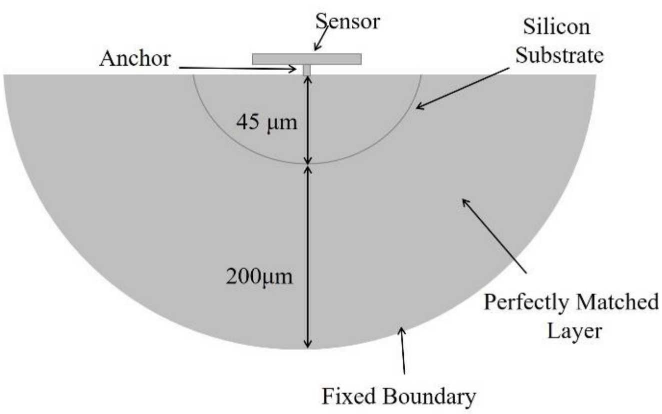

Fig. 5. Modeling of anchor loss using PML.

Regarding anchor loss, when the proposed sensor vibrates parallel to the substrate, acoustic waves propagate from the central anchor to the substrate, so the mechanical energy decrease. This phenomenon, a part of other damping sources, is studied through simulation using COMSOL Multiphysics under condition shown in Fig. 5 where a perfectly matched layer (PML) to absorb

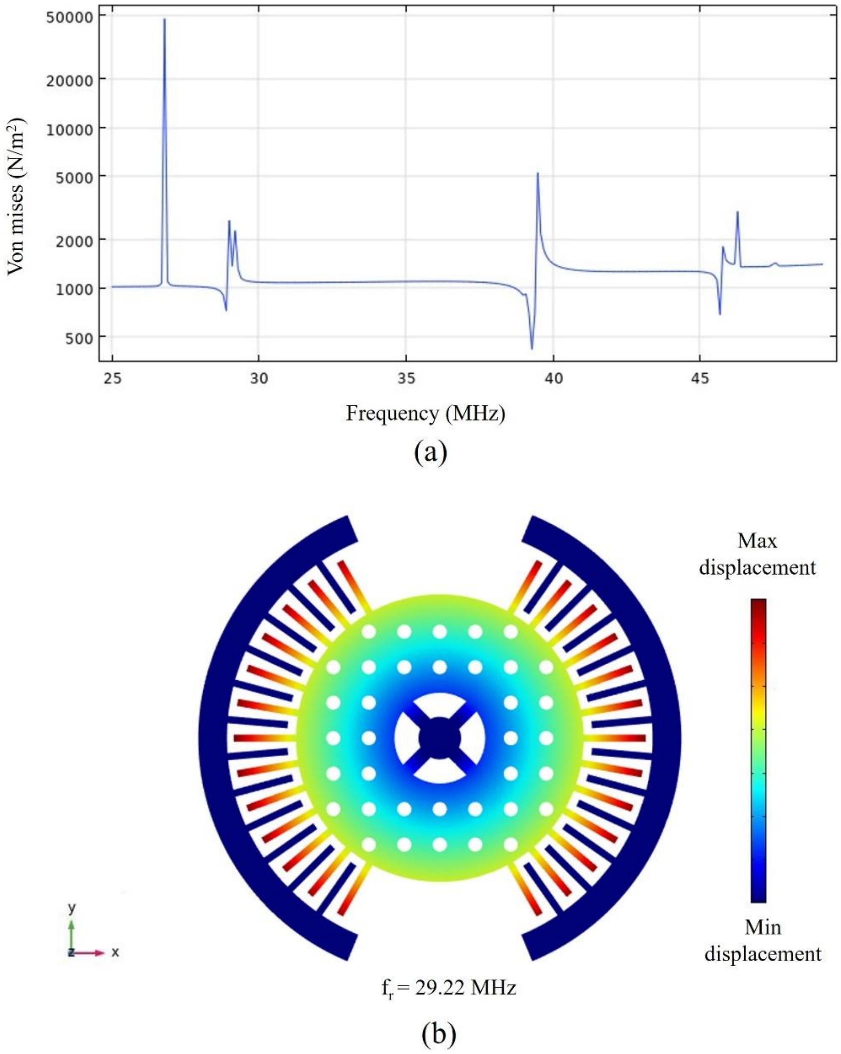

Fig. 6. (a) Different natural frequencies of the sensor and (b) Desired mode shape of the sensor at f=29.22 MHz.

Table 2. Material properties in the structural simulation.

Parameter	Value
Dynamic viscosity of the mercury	16e-6 (N·s/m^2)
Density of polysilicon	2320 (kg/m^3)
Young's modulus of polysilicon	160e9 (Pa)
Poisson's number of polysilicon	0.22

wave propagation within the substrate.

As the introduced sensor is designed to detect mercury particles, the mass sensitivity is a crucial parameter that should be assessed. The frequency shifts resulted from the added mass on the reaction area to the detected mass is defined as a mass sensitivity factor which follows [43]:

$$S = \left|\frac{\Delta f_0}{\Delta m}\right| \quad (4)$$

Δf_0 is the resonance frequency shift, f_0 is the working frequency, and Δm is the added target mass.

RESULTS AND DISCUSSION

Finite element method was used to study the proposed sensor structurally in a 3D environment. Performance characteristics of the system was extruded by solid mechanics physics in the COMSOL Multiphysics including natural resonance frequency, frequency response, quality factor, and mass sensitivity. All required specifications used in the simulation are listed in Table 2.

Natural frequencies

To obtain natural resonance frequency, eigen frequency study was done regarding zero displacement condition for the central anchor (u=v=w=0) of the proposed sensor. According to Fig. 1a, there are a lot of resonance frequency that the structure moves in various mode shapes, so the desired modes shape with frequency of *29.22 MHz* is where the sensor vibrate parallel to the substrate around the z-axis as the Fig. 1b.

Anchor loss

A spherical substrate with a perfectly matched layer (PML) was assumed to simulate the anchor loss. As Fig. 7 illustrates, the wave propagation from the anchor is absorbed by the perfectly matched layer. Using eigen frequency analysis through solid mechanics physics and under the mentioned condition, the quality factor of a resonator is 2e4 which is defined as the ratio of the real and imaginary components of its eigenvalue. Considering this high quality factor, it seems that the viscous damping is likely to be the dominant damping source in the sensor.

Frequency response

The structural analysis is done around the resonance frequency of the nanosensor with the boundary conditions of the slip wall boundary and shear and vertical forces at the bottom and top of the sensor, respectively. The displacement value at a point on the sensor is used to represent frequency response and mass shown in Fig. 8. In fact, by applying proper electrostatic force from the actuators to the central oscillator, the sensor begins to vibrate, and with the settling of the mercury vapor in the gold-coated sensing area, the resonance frequency decreases.

Fig. 8a illustrates the frequency response of

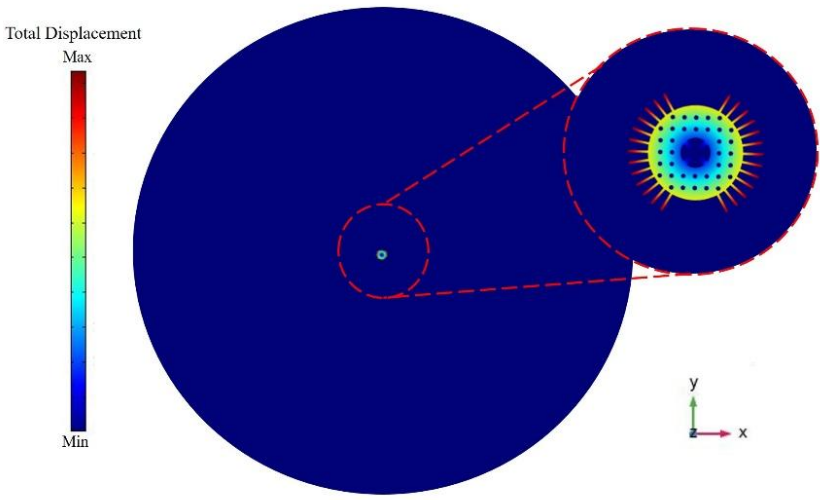

Fig. 7. Model shape of the sensor with PML at the frequency of 29.22 MHz.

the sensor which has two peaks, at frequencies of *29.206 MHz* and *29.246 MHz*, respectively. Considering the small size of the structure and the expectation of high operating frequency for the sensor, the results confirm that at the resonance frequency of *29.22 MHz*, the quality factor of the sensor resulted from viscous damping is approximately equal to *730* which is the ratio of the resonance frequency to frequency difference of the mentioned two peaks [44]. In comparing the

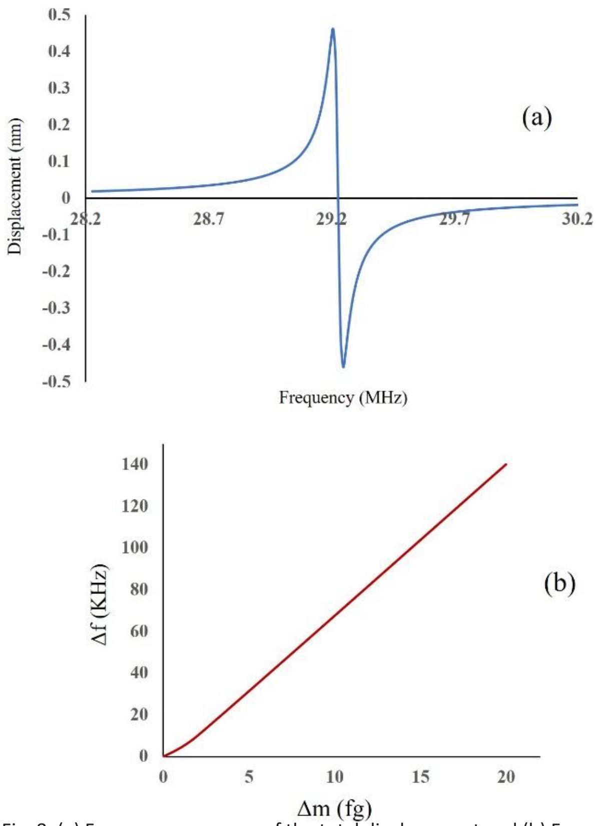

Fig. 8. (a) Frequency response of the total displacement and (b) Frequency shift of the sensor vs. absorbed mass.

Table 3. Comparison of the present study with similar mercury sensors.

Reference	Mercury concentration	Limit of detection (LOD)	Sensing method
[45]	0.1–1.0 ng/mL	NA	Chemoresistivty
[46]	61 -270 μg/m^3	16 μg/m^3	Colorimetric
[47]	< 1000 ng/m3	NA	-
[48]	< 400 ppb	2.6 ppb	SAW
[49]	0.5 -9.1 mg/m^3	35 μg/m^3	Conductometry
[50]	10.55 mg/m^3	NA	Frequency shift (QCM)
Present work	0.66-6 g/m^3	NA	Frequency shift

* N/A: Not reported

quality factor of anchor loss with viscous damping, the total quality factor of the sensor is almost *730*. Due to the very small gap between the sensor and the substrate and the resulting viscous resistance to sensor movement, this low value for the quality factor is acceptable.

To determine the mass sensitivity profile of the sensor, different concentrations of the target were applied to the simulation and the finite element results indicate that by increasing 1 ag of mercury concentration on the reaction area, the resonance frequency decreased to *7 Hz*, as shown in Fig. 8b. This value of sensitivity is reasonable because in design of the sensor, on both sides of the resonator, a sensitive material to mercury was assumed.

This high mass sensitivity makes the sensor detect mercury precisely in low concertation for environmental pollution and clean energy applications.

The results obtained from the simulation are significant and can potentially be used for the detection of mercury vapor in environmental pollution and clean energy applications. In Table 3, a comparison between the proposed sensor and similar cases is made. Based on the finite element and analytical results, the proposed mercury sensor is comparable to the experimental data provided by reported research.

CONCLUSION

In this research, a highly sensitive nanosensor was designed to trace mercury vapor as a toxic pollutant in environmental issues. Electrostatic actuators are used to drive the active area and capacitive sensing method is used to measure target particle through frequency changes. The innovation of this system is the use of gold on both sides of the sensor, which increases sensitivity as obtained in finite element-based simulation results. Additionally, the whole structure rotates around the z axis and parallel to the substrate, which reduces the damping effect on the performance. The results of structural simulation in solid-state mechanics of the COMSOL Multiphysics tool and analytical approach show that this sensor detects mercury in the picogram range at a frequency of 29.22 MHz. In addition, the proposed sensor is capable to detect mercury particles in the environment in real-time state without using extra nanomaterial, labels and complicated sensing equipment.

ACKNOWLEDGEMENT

This research is supported by the research grant of the University of Bonab (Grant Number 1402/P/01).

CONFILICTS OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this manuscript.

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