Design and modelling of a MEMS for detection of volatile organic compound

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Abstract. Volatile organic compounds pollute air in and out of homes, which effects human health when inhaled. It is necessary to monitor these gases with rapid response sensors at low concentrations, such as with electromechanical systems. We designed and simulated of a multilayer cantilever sensor using finite element method, which is 3 mm long, 2 mm wide, and 52.2 µm thick, activated with the piezoelectric effect with a zinc oxide film and a titanium oxide film that is sensitive to gases. The first resonance frequencies were obtained with modal analysis using ANSYS®, in which the first frequency is 4722.4 Hz, the minimum sensitivity of the multilayer gas sensor is 8.22 kHz/g and a minimum detectable mass change ($\Delta m_c$) of 2432.32 ng. This sensor could be used in industry or in homes.

1. Introduction

Air pollution is mainly caused by volatile organic compounds (VOCs), which damage both short-term and long-term human health. Developing nations have an unfair burden in terms of air pollution that causes 4.2 million premature deaths, which reflects the importance of a VOC-free environment. Non-transmissible illnesses will decrease with a reduction in exposure to environments polluted with VOCs. Outdoor air pollution is not the only concern we should have, pollution in homes caused 4.3 million premature deaths in low to medium income countries in 2012 [1].

For VOC-free environments, it is necessary to have gas sensors. Microelectromechanical systems (MEMS) are used as gas sensors to monitor for low concentrations of VOCs, they have low power consumption, are light, small, and have a low cost when they are mass produced. The cantilever structure is the most commonly used as a MEMS gas sensor due to its large out of plane displacement [2]. This structure can be manufactured with materials such as silicone, polysilicon, polymers, and metals [3]. The structure can be activated with resistive, capacitive, or piezoelectric methods [4]. Zinc oxide (ZnO) is used as a piezoelectric layer to activate the MEMS sensors, which is compatible with manufacturing processes [5]. Anatase phase titanium dioxide (TiO₂) films can be used as a layer sensitive to VOCs in a gaseous state [6]. We propose a MEMS gas sensor with a cantilever structure that is activated with...
piezoelectricity in order to detect VOCs. This sensor was designed and simulated using the finite element method (FEM), which consists of a 304 stainless steel substrate (50 µm thick), 2 aluminum contacts (100 µm thick), a ZnO piezoelectric film (1 µm thick), and a TiO$_2$ film which is sensitive to VOCs (1 µm thick) (Figure 1).

![Figure 1. Side view of the MEMS multilayer gas sensor.](image)

2. Materials and Methods
This section presents the modeling of a MEMS multilayer sensor that obtains a resonance frequency using the finite element method (FEM).

2.1. Design
Figure 2 shows the multilayer gas sensor was designed in Solidworks®, which has a length (l) of 3 mm and a width (b) of 1 mm, the sensor layers are the same length and width. 304 AISI stainless steel, 50 µm thick, was used as a substrate and had a low cost. A 1 µm thick zinc oxide piezoelectric film between two 100 nm thick aluminum contacts, two 100 nm thick aluminum pads for circuit connection, and finally a 1 µm thick titanium dioxide film sensitive to VOCs was also used.

![Figure 2. MEMS multilayer gas sensor schematic.](image)

The resonant frequency of the cantilever is represented as follow, [7].

\[
 f_r = \frac{1}{2\pi} \sqrt{\frac{k}{m}} \tag{1}
\]

Where \( k \) is the spring constant and \( m \) is the effective mass of the cantilever. To calculate the sensitivity of the gas sensor MEMS to the interaction of VOCs is calculated by equation 2. With the resonance
frequency, is possible to calculate the minimum mass who detects the gas sensor that can be calculated by the following equation 3.

\[ sensibility = \frac{\Delta f}{f_r} \]  \hspace{2cm} (2)

\[ \Delta m_c = 2m_e \frac{\Delta f}{f_r} \]  \hspace{2cm} (3)

\( m_e \) the mass of the gas sensor, \( \Delta f \) it’s change of frequency, \( f_r \) the resonant frequency of the cantilever. The resonant frequency decreases when adding the change in mass, to calculate this change in frequency with the detection of VOCs, the change in mass is added to equation (1), resulting in equation (4).

\[ f_r = \frac{1}{2\pi} \sqrt{\frac{k}{m_e + \Delta m_c}} \]  \hspace{2cm} (4)

2.2. Finite Element Method

Modal analysis with the finite element method (FEM) was performed with the design of the MEMS gas sensor, in which aluminium contacts were not rejected. Table 1 shows the properties of isotropic materials used for this analysis [8-16]. Figure 3 shows the mesh used for the gas sensor model developed in ANSYS® with 2100 elements and 12020 nodes.

| Layer | Material   | Young’s modulus (Pa) | Poisson ratio | Density (km/m³) |
|-------|------------|----------------------|---------------|-----------------|
| 1     | Stainless steel 304 | 2 x 10¹¹           | 0.29          | 8000            |
| 2,4   | Al         | 7 x 10¹⁰           | 0.331         | 2700            |
| 3     | ZnO        | 1.37 x 10¹¹        | 0.25          | 5665            |
| 5     | TiO₂       | 1.51 x 10¹¹        | 0.27          | 3840            |

Table 1. Properties of the isotropic materials used for the gas sensor [8-16].

Figure 3. MEMS multilayer gas sensor grid.
3. Results
The cantilever was anchored at one end and free at the other end using modal analysis with the MEMS multilayer gas sensor. Using a FEM model, the four modes of vibration were obtained (Figure 4). The first vibration mode has a resonance frequency of 4722.4 Hz and is a bending mode (Figure 4a). The second and third vibration modes (Figures 4b, c) respectively have frequencies of 28858 and 29476 Hz. Finally, the fourth vibration mode (Figure 4d) has a frequency of 82591 Hz and registers irregular displacements, Table 2 shows the frequency and maximum deformation the MEMS multilayer gas sensor.

![Figure 4](image)

**Figure 4.** First four vibration modes of the MEMS multilayer gas sensor: (a) first (4722.4 Hz), (b) second (28858 Hz), (c) third (29476 Hz), and (d) fourth (82591 Hz).

The resonance frequencies then associated with the VOCs in a gaseous phase. We are interested in the first vibration phase, which is directly associated with the displacement of the percentage of VOCs.

| Frequency (Hz) | Deformation (µm) |
|---------------|------------------|
| 4722.4        | 1809.7           |
| 28858         | 2335.6           |
| 29476         | 1818.2           |
| 82591         | 1858.6           |

The analytical resonance frequency was calculated with the values in Table 1 obtaining 4774.1 Hz. When comparing the first analytical resonance frequency with that obtained in the FEM model, an error of 1.08 % was obtained. The minimum sensitivity of the multilayer gas sensor is 8.22 kHz/g and a minimum detectable mass change ($\Delta m_c$) of 2432.32 ng. A harmonic response analysis was performed with air and with distributed masses, where the quality factor of 3403.305 and a damping ratio of 0.00014692 were considered. The figure 5 show displacement vs frequency in the function the VOC’s mass.
4. Conclusions
This study presents the design of a multilayer gas sensor with a cantilever structure. The microsensor is made up of an AISI 304 stainless steel substrate, which has mechanical properties that are similar to silicone, but costs less. The first resonance frequency of the multilayer gas sensor was determined to be 4.72 kHz, when comparing the analytical resonance frequency with that obtained in the FEM model, an error of 1.08% was obtained. The minimum sensitivity of the multilayer gas sensor is 8.22 kHz/g and a minimum detectable mass change ($\Delta m_c$) of 2432.32 ng, this frequency will make it possible to associate changes in frequency with changes in gas concentrations. The multilayer gas sensor could be used in industries and homes and be monitor the presence of VOCs in real time and at room temperature and help to reduce respiratory illnesses and have a clean environment.

We plan to study sensibility and selectivity with the finite element method in the future, as well as the maximum displacement associated with resonance frequency.

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