Effect of Substrate Material on Sensing Behaviour of SAW Based Gas Sensors

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Abstract. In this paper, we have designed a SAW gas sensor based on MEMS technology to detect volatile organic gases. Finite element analysis of the device had been carried out to observe the changes in the sensor behaviour with the applied gases. Also, the designed SAW Gas Sensor is analysed with different piezoelectric substrate. Lithium Tantalate is found to be best suited for the design which defines the resonant frequency of the device to be approximately 1.184 GHz. The device is further simulated with different volatile organic gases which give corresponding shift in frequency.

INTRODUCTION

MEMS or Micro-Electro-Mechanical System is a technology that has the potential to bring revolution to industries and various products that can be made by incorporating electrical as well as mechanical components on a single chip. It is recognized as one of the most favourable technologies to change the current scenario of this century by developing devices of size varying from few millimetres to micrometres. They have the capability to actuate, control and sense on micro level and produce results on macro level.

Surface Acoustic Waves or SAWs are those mechanical waves which travel along the surface of an elastic material [1-3]. This wave also known as Rayleigh wave possesses velocity ranging from 1000 m/s to 15000 m/s. This velocity known as Rayleigh Wave velocity varies from material to material along which they travel [4-6]. Surface acoustic wave's velocity is quite lesser than EM waves which give an advantage to designer who incorporates these waves instead of EM waves to design devices of size of few micrometres [7-10]. The amplitude of these waves dies with the depth of the substrate exponentially.

Gas sensing by SAW sensors is reported widely in literature. Gases like CO_2, H_2S, Dichloromethane, LPG, CH_4, CO, H_2, NO and so on. The sensing layer of the SAW sensor plays an important role in sensing of these gases. Technology is developed to sense these gases up to parts per million.

In this paper the authors have investigated the effect of substrate material on the sensing behaviour of the SAW sensor. Different substrate materials like Cadmium Sulfide, Lithium Tantalate, Lithium Niobate, Zinc Oxide and Lead Zirconate Titanate have been used to analyse the performance of the SAW sensor. Lithium Tantalate is found to be best suited for the design which defines the resonant frequency of the device to be approximately 1.184 GHz. The device is further simulated with different volatile organic gases which give corresponding shift in frequency.

DEVICE STRUCTURE

Figure 1 shows the 3D geometry of a typical SAW Gas Sensor. It consists of three parts: Piezoelectric substrate, InterDigital Transducer (IDT) and a Sensing Layer. Input IDT are provided with electrical signal of a particular frequency called as resonant frequency of device which is calculated from Rayleigh wave velocity, hence it depends on piezoelectric substrate. After the application of RF voltage corresponding to resonant frequency, electric field lines are generated in IDT which causes stress due to piezoelectric effect as IDT is layered upon piezoelectric substrate. Stress produced give rise to surface acoustic waves [5]. These waves are easily influenced by the gas present on the surface. The SAWs are then converted into electrical signal on output IDT due to piezoelectric effect. The frequency detected is lower than the resonant frequency and shift is called as frequency shift [6].

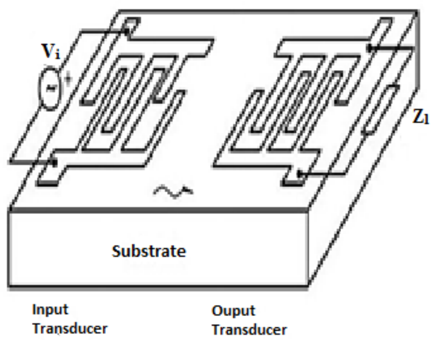


FIGURE 1. Basic Structure of SAW Gas Sensor

2D structure of SAW Gas Sensor is simulated in COMSOL as shown in figure 2. The 3D geometry of SAW sensor is compressed into a unit cell. This is possible because IDT consist of many similar electrodes with their length being 100 times of their width in a comb like fashion. Due to such geometry of IDT, edge effect can be neglected and hence periodic condition are applied to vertical boundary of the unit cell to determine electric potential and displacement within the device.

The substrate of the proposed structure is 2.8µm wide and 8.5µm in length. Five different piezoelectric substrates are analysed for this geometry. The electrodes of IDT rest on substrate, made of aluminium of width 0.7µm and height 0.2µm. Electrodes are covered with a thin sensing film of Poly-iso-butylene (PIB) of thickness 0.5µm and 2.8µm wide.

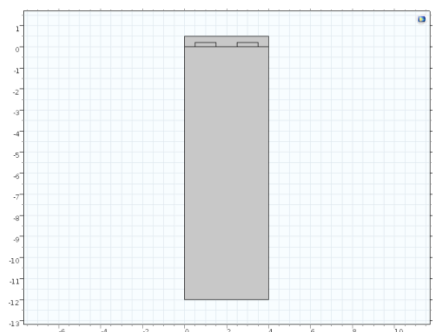


FIGURE 2. 2D structure of SAW Gas Sensor

SIMULATION METHODOLOGY

Periodic conditions are applied on vertical boundaries of unit cell. This implies that the wavelength of the wave must be an integer fraction of the width of unit cell. The RF voltage corresponding to resonant frequency of device is calculated from Equation (1).

$$f = vR/width \tag{1}$$

Where, f is Resonant frequency of device vR is Rayleigh Wave Velocity and *width* is width of unit cell.

When the device is exposed to air, the density of the PIB film increases. The partial density of PIB is calculated by following equations

$$\rho DCM, PIB = KMC \tag{2}$$

$$C = (c0.10^{-6}.p)/RT \tag{3}$$

$$K = 10^{a} \tag{4}$$

Where, a is Air/PIB partition coefficient of particular gas, c0 is the concentration in parts per million, p is the pressure, T is the temperature, R is the gas constant, M is the molar mass of particular gas.

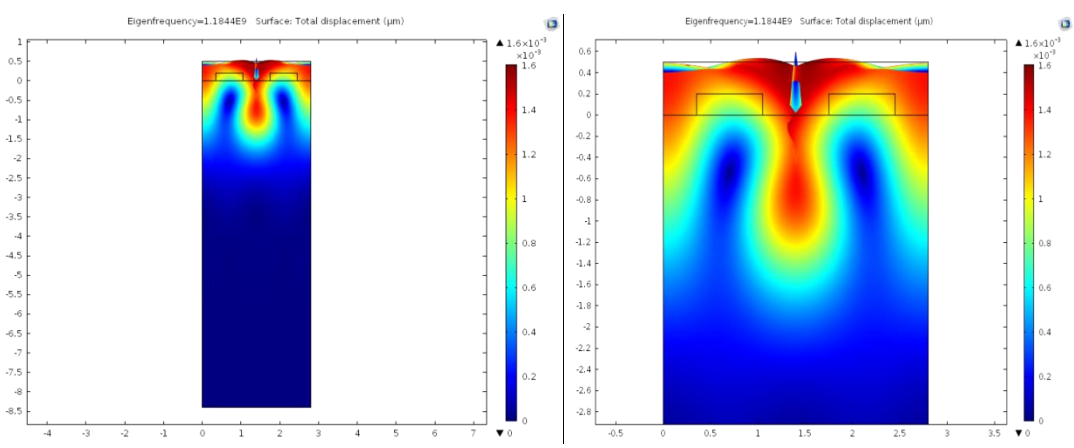
RESULTS AND DISCUSSION

The device is analyzed with 5 piezoelectric substrate: Cadmium Sulfide, Lithium Tantalate, Lithium Niobate, Zinc Oxide and Lead Zirconate Titanate. The Rayleigh wave velocity of different substrate is different which defines unique resonant frequency for device to work on. This frequency is calculated from Equation (1). The device is exposed to air containing 100 ppm Di-Chloro-Methane.

TABLE 1. Frequency Shift of SAW for different piezoelectric substrate for Di-Chloro-Methane Gas

Piezoelectric Substrate	Rayleigh Wave Velocity (m/s)	Resonant Frequency (Before exposure to Gas =A) ($\times 10^{9}$ Hz)	Resonant Frequency (After exposure to Gas =B) ($\times 10^{9}$ Hz)	Frequency Shift = A-B (Hz)
Lithium Niobate	3844	1.205859455329653	1.205859145729650	309.60
Lithium Tantalate	3230	1.184449310731556	1.184448942337684	368.39
Cadmium Sulfide	1700	0.582484614317719	0.582484549953261	64.36
Zinc Oxide	2600	0.954955326614580	0.954955133157525	193.46
Lead Zirconate Titanate	2100	0.805776221725167	0.805776006942410	214.78

As mentioned in the table 1, Lithium Tantalate gives highest frequency shift while Cadmium Sulfide shows lowest shift in frequency. Lithium Tantalate is cheaper than the rest and being more sensitive towards the gas as frequency shift is highest comparatively, chosen to be best suited as a substrate for the designed proposed. Figure 3 and 4 shows the displacement and electrical plots of device when exposed to DCM with Lithium Tantalate as substrate with resonant frequency 1.184 GHz.



(a) (b)

FIGURE 3. Deformed plots

From figure 3 (a) it can be observed there is no displacement in the device with depth of the substrate and the maximum displacement in the device due to surface acoustic waves is near the electrodes and on its surface

Figure 4 shows the electric potential distribution in the device. It is symmetric with respect to the centre of electrodes.

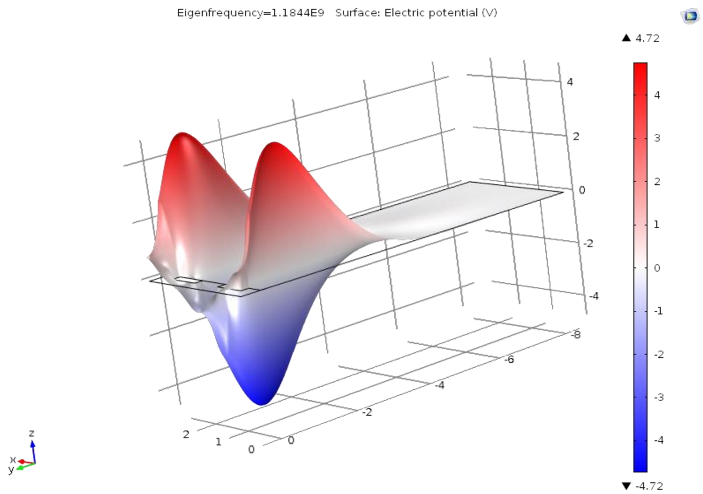


FIGURE 4. Electric Potential Distribution in device

TABLE 2. Frequency Shift of SAW for different organic gases with Lithium Tantalate as substrate

Gas	Resonant Frequency (Before exposure to Gas =A) (× 10^9 Hz)	Resonant Frequency (After exposure to Gas =B) (× 10^9 Hz)	Frequency Shift = A-B (Hz)
Chloromethane	1.18444493107315564	1.1844492849457655	25.79
Di-Chloromethane	1.18444493107315564	1.1844489423376840	368.39
Tri-Chloromethane	1.18444493107315564	1.1844478658790538	1444.85
Carbon Tetra-chloride	1.18444493107315564	1.1844457779209130	3532.81
Tetra-Chloroethene	1.18444493107315564	1.1844266785958393	22632.14
Tetra-Chloroethylen	1.18444493107315564	1.1844445991779017	4711.55

The device with Lithium Tantalate as substrate is exposed to various volatile organic gases. As shown in Table 2, Chloromethane gives lowest shift in frequency while Tetra-Chloroethene gives the highest.

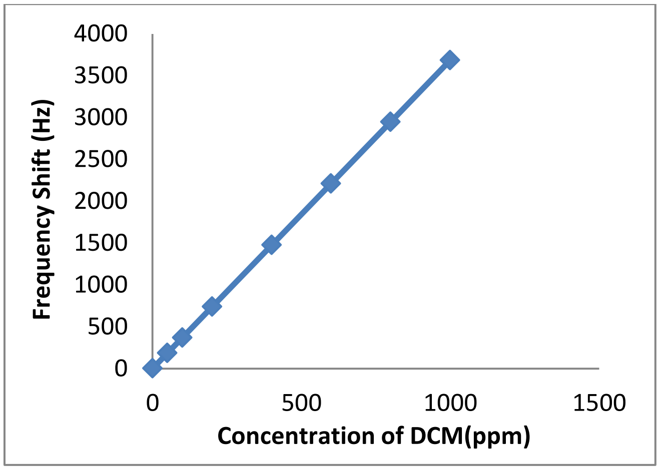


FIGURE 5. Frequency Shift vs Concentration of DCM

Figure: 5 shows the relation between frequency shift and the concentration of DCM in air. It can be clearly observed from the plot that shift in frequency increases with increase in concentration of gas in air.

Figure 6 shows the effect of thickness of sensing layer on the frequency shift. As can be seen from the plot, if we increase the thickness of PIB, shift in frequency also increases.

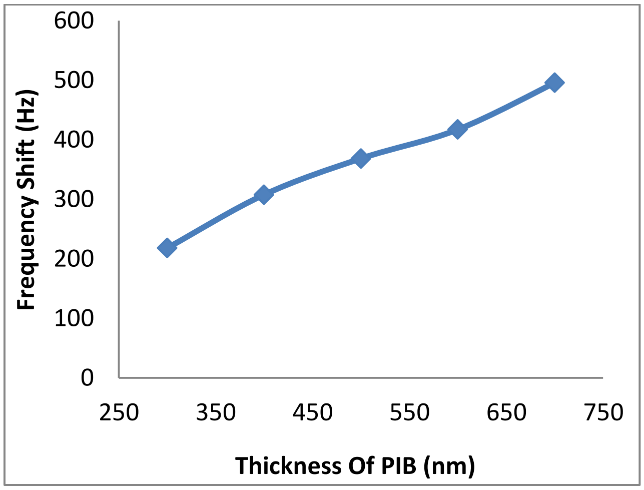


FIGURE 6. Frequency Shift vs Thickness of PIB

CONCLUSION

The design proposed for SAW Gas Sensor is analysed with five different piezoelectric substrate. Lithium Tantalate is found suitable for the design with SAW resonant frequency of 1.1844 GHz. The sensor is simulated by exposing it to various volatile organic gases which causes corresponding shift in frequency [10]. These volatile gas have low boiling point and high vapour pressure at room temperature which causes them to vaporize in surroundings and pollutes the environment [4] [9]. Such sensors can be used in industries to estimate the concentration of organic gases.

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