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Design and Analysis of SAW Based MEMS Gas Sensor for the Detection of Volatile Organic Gases

Staline Johnson*, Dr. T. Shanmuganantham **
*(Department of Electronics Engineering, Pondicherry University, Puducherry)
** (Department of Electronics Engineering, Pondicherry University, Puducherry)

ABSTRACT
This paper portrays the design and analysis of SAW based MEMS gas sensor for the detection of volatile organic gases. The gas sensor consists of interdigitated transducers modeled on a piezoelectric substrate and covered by a thin film of polyisobutylene (PIB) which acts as the sensing layer. The piezoelectric substrate material used is YZ cut Lithium Niobate (LiNbO3) and electrodes used are made of Aluminium (Al). Mass loading effect on the sensing layer is used for the detection of volatile organic gases. The design and simultions were carried out by using comsol multiphysics software based on Finite Element Method (FEM) for analytical simulations. The resonant frequency of the SAW device was determined and simulations are carried out by exposing the sensor to 100 ppm of various volatile organic gases and corresponding shift in resonant frequency for various gases are determined. The reduction in the resonant frequency is used for the detection of volatile organic gases such as chloromethane, dichloromethane, trichloromethane, tetrachloroethene, carbon tetrachloride and trichloroethylene.
***Keywords* -** Comsol Multiphysics, gas sensor, MEMS, piezoelectric, surface acoustic waves.

I. INTRODUCTION

Surface acoustic wave is a mechanical wave propagating along the surface of a piezoelectric material and its amplitude decreases exponentially with the depth of the material. Surface acoustic waves are employed in electronic devices such as sensors, actuators, filters, and oscillators [1][2]. Surface acoustic wave sensors are a part of microelectromechanical systems which senses a physical phenomenon by modulation of surface acoustic wave. The surface acoustic wave gas sensor consist of an input interdigitated transducer[IDT] and output IDT etched on a piezoelectric substrate covered with thin sensing film. The input IDT converts electrical signal to surface acoustic wave and output IDT converts back to electrical output signal. The sinusoidal electrical input signal to a piezoelectric acoustic wave sensor, causes alternating polarity between adjacent electrodes.This alternating electricfield creates alternating regions of tensile and compressive strain due to piezoelectric effect. As a result a mechanical wave is generated at the surface known as surface acoustic wave [3]. Volatile organic compounds are those chemicals which which are having high vapour pressure at room temperature due to low boiling point. This low boiling point causes it to evopaorate to the surrounding air causing health hazards for humans and pollute the environment [4].

The analytical simulation of the proposed model was done by using Comsol Multiphysics software which is a commercial finite element tool for analysing the model. The material used for piezoelectric substrate is YZ cut Lithium niobate and is having high saw velocity when compared to other piezoelectric materials such as quartz and lithium tantalate [5][6].The interdigitated tranducers are made of aluminium and sensing layer used is polyisobutylene film. Polyisobutylene is a polymer thin film having high affinity towards volatile organic gases.It is a rubbery material with a Poisson’s ratio of 0.48 and Young’s modulus of 10GPa. SAW chemical sensors works on the variations of the SAW phase velocity and attenuation of the surace acoustic wave as the vapor adsorbed on the sensing film. The sensing film is a chemicalcompound that selectively and reversibly interacts with the analyte vapor [7][8]. Air is taken as reference gas and resonant frequency of the saw gas sensor is determined when exposed to air.When the saw gas sensor is exposed to 100 ppm of gas in air which results in the reduction of the resonant frequency. This is because the density of polyisobutylene will increase due to absorption of the gas. The shift in the resonant frequency is due to mass loading effect on the sensing layer [9]. When the polymer absorbs an analyte, its mass increases and density of the sensing film also changes. This additional mass on the substrate will decrease the velocity of mechanical waves propagating through the substrate, which corresponds to a phase change in the electric signal generated at the output transducer. The shift in the resonant frequency is determined by mixing the signal from the sensor when expose to air i.e reference signal with signal when exposed to gas, the beat frequency gives the shift. The main applications of gas sensors includes process control industries, electronic noses, fire detection and home safety [10].

II. SENSOR STRUCTURE

The proposed geometry of saw gas sensor is shown in Figure 1. The interdigitated transducers used in saw devices consist of many identical electrodes and the length of the electrode is made 100 times the width to eliminate edge effects. Therefore modeled geometry is reduced to a periodic unit cell. The height of the cell is designed in such a way that at the saw almost died at the lower boundary. The substrate is made of piezoelectric material yz cut lithium niobate having a width of 3 µm and height of 17.5 µm. The electrodes used are made of aluminium having a width of 0.75 µm and height of 0.1 µm. The sensing thin film is having a width of 3 µm and height of 0.5 µm. The operating frequency of the saw device is 1.121 GHz.

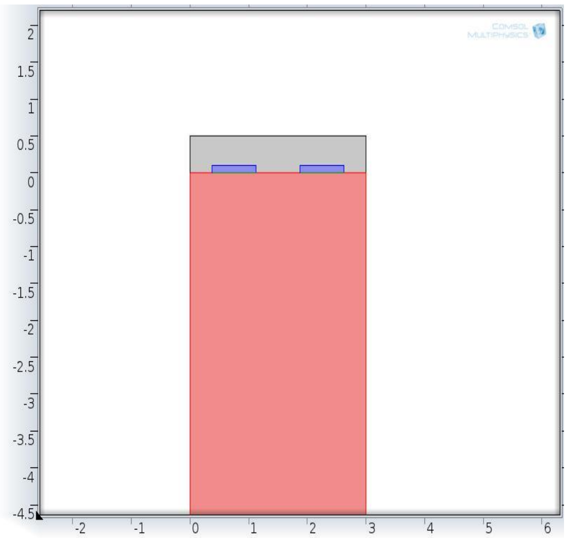

Figure 1: Proposed design of the gas sensor (all dimensions are in µm)

III. DESIGN PARAMETERS

The absorption of gas by the polyisobutylene film is indicated as an increase in the density of the film. The density of the film is 0.918g/m^3 []. The Poison's ratio is set to 0.48, Young's modulus to 10GPa and relative permittivity to 2.2. The width of the model is fixed at 3 µm so that lowest Eigen mode has a wavelength equal to width of the geometry. Hence we can evaluate saw velocity. The sensor is exposed to 100 ppm of various volatile organic gases at standard temperature and pressure. The concentration of gas in air (c) is evaluated using the following equation 1.

$$c = (100 \times 10^{-6} \times P)/RT \qquad (1)$$

Where P is the air pressure, R is the gas constant and T is the air temperature.

$$\rho_{gas/PIB} = KMc \qquad (2)$$

Equation 2 gives the partial density of absorbed gas in the polyisobutylene film. K is the air/PIB partition coefficient for the gas [5], M is the molar mass of the gas and c is the concentration of gas in air.

$$\rho_{total} = \rho_{PIB} + \rho_{gas/PIB} \qquad (3)$$

The above equation gives the total density of PIB due to gas absorption. ρ_{PIB} is the density of PIB film and $\rho_{gas/PIB}$ is the partial density of gas in air.

$$\frac{\Delta f_m}{f_0} = \frac{\Delta v_m}{v_0} = -Kf_0 h[K_1(\rho) + K_2(\rho) + K_3\left(\rho - \frac{4\mu(\lambda+\mu)}{v_0^2(\lambda+2\mu)}\right) \qquad (4)$$

The shift in the resonant frequency due to mass loading effect is given by equation 4 [2]. Where f_0 represents the operating frequency, h is the film thickness, Ki is the normalized particle velocities in the xi direction, ρ is the film density, v_0 is the nominal saw velocity, λ and µ are Lame constants of the film.

TABLE I: partial densities of absorbed gases in the film

Gas	K[5]	M[5]	$\rho_{gas/PIB}$ (Kg/m^3)
Chloromethane	0.5538	50.4	7.3589$\times 10^{-4}$
Dichloromethane	1.4821	85.0	0.010534
Trichloromethane	1.9273	119.5	0.041316
Carbon tetrachloride	2.2060	153.8	0.10102
Tetrachloroethene	2.9799	165.8	0.16583
Trichloroethylene	2.3994	131.4	0.13472

Table 1 gives the values of air/PIB partition coefficient and molar mass of various gases thereby we can evaluate the partial density of absorbed gas in PIB film.

IV. RESULTS AND DISSCUSION

The resonance and anti-resonance frequency was evaluated to be 1.121 GHz and 1.131 GHz. The IDT electrodes and sensing film polyisobutylene causes the lowest saw mode to split up into two Eigen solutions. The lowest frequency represents the resonant mode frequency in which propagating waves interfere constructively. The other one represents the anti-resonance frequency in which propagating waves interfere destructively. Waves do not propagate with in these two frequencies and it represents the edges of stop band.

TABLE 2: Simulation results of shift in resonance frequency when exposed to various gases

Gas	$\frac{\rho_{gas}}{\rho_{PIB}}$ (Kg/m³)	f_r (Hz)	Δf_r(Hz)
Air (reference gas)	0	1121215 325	------
Chloromethane	7.3589 $\times 10^{-4}$	1121215 300	25
Dichloromethane	0.010534	1121214 969	356
Trichloromethane	0.041316	1121213 931	1394
Carbon tetrachloride	0.10102	1121211 917	3408
Tetrachloroethene	0.16583	1121193 494	21831
Trichloroethylene	0.13472	1121210 781	4544

Table 2 shows the shift in the resonant frequency (Δf_r) when the saw gas sensor is exposed to 100 ppm of various gases at atmospheric pressure and temperature. Simulations are done using Comsol Multiphysics software, a finite element method based tool to analyse the model. Air is taken as reference gas and the resonant frequency of the saw gas sensor is evaluated. The sensor is again exposed to 100 ppm of various gases and their resonant frequencies are evaluated. It is seen that there is a shift in the resonant frequency downwards when compared to the reference gas. The shift in the resonant frequency is because of the increase in the density of the polyisobutylene film due to absorption of gas by the film. Thereby we can detect the gas using the shift in the resonant frequency. Change in the resonant frequency due to change in the density of the sensing layer due to absorbed gas is used for detection of various gases.

Gas	Sensitivity (Hz/ Kgm^{-3})	Gas	Sensitivity (Hz/ Kgm^{-3})
Chloromethane	33972	Carbon tetrachloride	33735
Dichloromethane	33794	Tetrachloroethene	131646
Trichloromethane	33739	Trichloroethylene	33729

Table 3 shows the sensitivity comparison of various gases at 100 ppm concentration of gas. Since the gases are having different partial densities, the shift in the resonance frequency will also be different and we are able to detect the gases. Sensitivity is the ratio of shift in the resonant frequency to partial density of the absorbed gas in the sensing film.

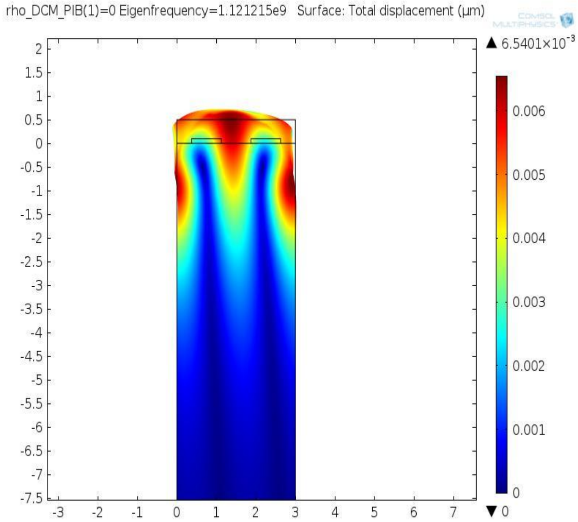

Figure2: Deformed plot showing saw resonance mode

Figure 2 shows the resonant saw mode with a resonant frequency of 1.121215325 GHz. Resonant saw mode occurs due to constructive interference of propagating waves. It is seen that most of the saw waves occur at the surface and its amplitude decreases with the depth of the material.

Figure 3 shows the anti-resonant saw mode with a resonant frequency of 1.131918619 GHz. Anti-resonant saw mode occurs due to destructive interference of propagating waves

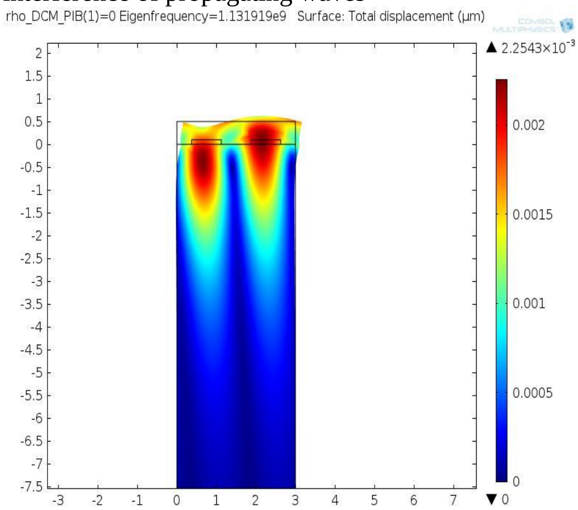

Figure3: Deformed plot showing saw anti-resonance mode

Figure 4 shows the electric potential distribution and deformation and is symmetric with respect to center of each electrode.

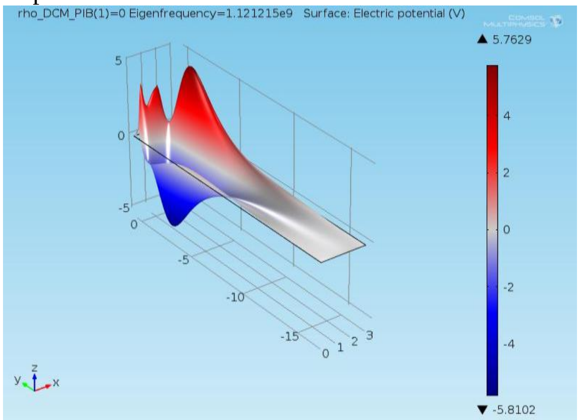

Figure4: Electric potential distribution at resonance

Figure 5 shows the electric potential distribution and deformation and is anti-symmetric with respect to center of each electrode.

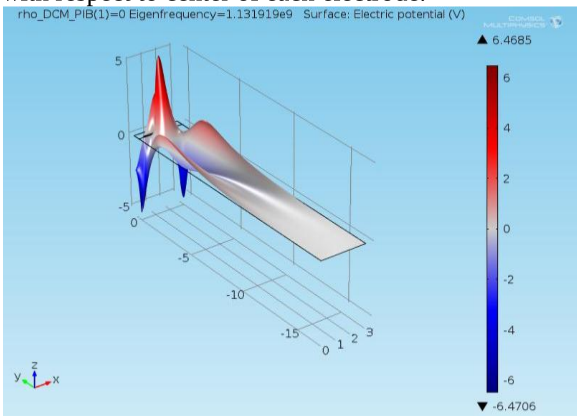

Figure5: Electric potential distribution at anti-resonance

Figure 6 shows the deformed plot of resonant saw mode with a resonant frequency of 1.121214969 GHz when exposed to 100 ppm of dichloromethane gas. It is seen that there is a shift in resonant frequency of 356 Hz downwards because of increase in the density of polyisobutylene film due to gas absorption. The partial density of the100 ppm of dichloromethane gas was found to be 0.010534 Kgm^{-3} and the shift in the resonant frequency is used for detection of various gases.

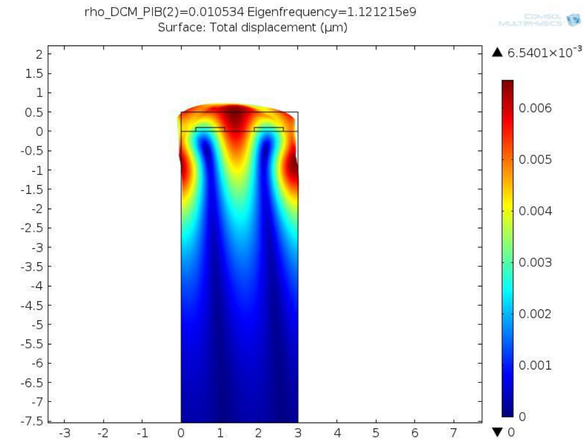

Figure6: Deformed plot showing saw resonance mode when exposed to 100 ppm of dichloromethane gas.

Figure 7 shows variation of total displacement at various frequencies. It is seen that maximum displacement of 6.5401$\times 10^{-6}$μm occurs at the resonant frequency.

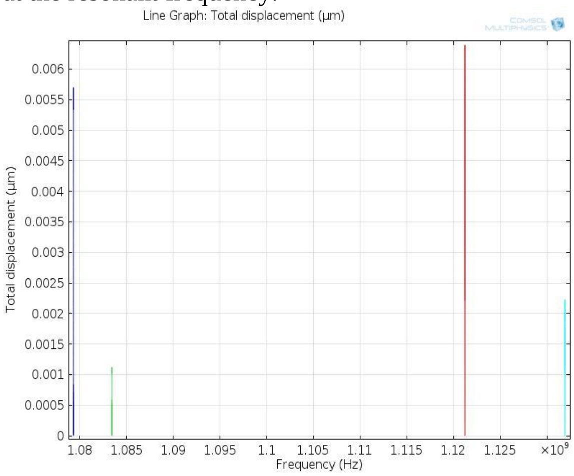

Figure7: Graph showing total displacement at various frequency

V. CONCLUSION

The surface acoustic wave based MEMS gas sensor was designed and the operating frequency of the saw device was found to be 1.121 GHz. The maximum sensitivity is obtained, since the gas sensor is operating in GHz range. The maximum shift in the resonant frequency is for tetrachloroethene because of maximum partial density of absorbed tetrachloroethene. As the partial density of absorbed gas increases the resonant frequency shift also increases. Saw gas sensor has the advantages of small size, low cost of fabrication, long life time, high sensitivity and selectivity. Saw gas sensor are mainly used for chemical industries, military applications and also used in wireless sensing applications.

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