Volatile Gas Detection using SAW based MEMS Device

BITS F415: Introduction to MEMS

Project Work

By

Nishant Jagtap
2018A4PS0510G

Project Work carried out by

TEAM F

Mayuresh Magdum	(2018A4PS0522G)
Nishant Jagtap	(2018A4PS0510G)
Shashank Sonpawale	(2018A4PS0533G)

BIRLA INSTITUTE OF TECHNOLOGY & SCIENCE
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Submitted in partial fulfillment of BITS F415 (Introduction to MEMS) course

Under supervision of
Dr. Devendra Patil

BIRLA INSTITUTE OF TECHNOLOGY & SCIENCE
PILANI (RAJASTHAN)
April 2021

DECLARATION BY THE STUDENT

I, **Mayuresh Vishwajeet Magdum** ______________________ hereby declare that the project report entitled "**Project Name**" submitted by me to BITS Pilani, KK Birla Goa Campus, in partial fulfilment of **BITS F415 (Introduction to MEMS) Sem. II AY 2020-21** course is a Bonafide report based on the work carried out by me and my **Team X** during the course of my study under the supervision of Dr. Devendra Gokul Patil.

My Contribution :

I have done the literature survey and collected the data. I have analysed the parameters that can be varied and collected the necessary information. We collectively compared the data and derived the conclusion.

I assure that the statements made and the conclusions drawn are an outcome of the project work. I further declare that to the best of my knowledge, the report does not contain any part of any work which has been submitted by someone else in any other publication.

Place: Pune, Maharashtra
Date: 27/04/2021

Signature of candidate :
Student Name : Mayuresh Magdum
Student ID : 2018A4PS0522G

DECLARATION BY THE STUDENT

I, **Nishant Nanasaheb Jagtap** hereby declare that the project report entitled "**Project Name**" submitted by me to BITS Pilani, KK Birla Goa Campus, in partial fulfilment of **BITS F415 (Introduction to MEMS) Sem. II AY 2020-21** course is a Bonafide report based on the work carried out by me and my **Team X** during the course of my study under the supervision of Dr. Devendra Gokul Patil.

My Contribution :

I went through various simulations and performed simulations for the study for varying electrodes shapes and varying gases. We collectively compared the data and derived the conclusion.

I assure that the statements made and the conclusions drawn are an outcome of the project work. I further declare that to the best of my knowledge, the report does not contain any part of any work which has been submitted by someone else in any other publication.

Place: Pune, Maharashtra
Date: 27/04/2021

Signature of candidate : 
Student Name : Nishant Jagtap
Student ID : 2018A4PS0510G

DECLARATION BY THE STUDENT

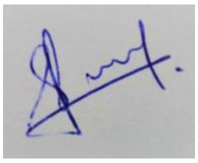
I, **Shashank Anil Sonpawale** hereby declare that the project report entitled "**Project Name**" submitted by me to BITS Pilani, KK Birla Goa Campus, in partial fulfilment of **BITS F415 (Introduction to MEMS) Sem. II AY 2020-21** course is a Bonafide report based on the work carried out by me and my **Team X** during the course of my study under the supervision of Dr. Devendra Gokul Patil.

My Contribution :

I have tried to extract results, prepare the excel sheets and analysed and organised the data. We collectively compared the data and derived the conclusion from the same.

I assure that the statements made and the conclusions drawn are an outcome of the project work. I further declare that to the best of my knowledge, the report does not contain any part of any work which has been submitted by someone else in any other publication.

Place: Selu, Parbhani, Maharashtra
Date: 27/04/2021

Signature of candidate : 
Student Name : Shashank Sonpawale
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Abstract

This project is about SAW based MEMS gas sensor which can be used to detect the gas leaks in industrial domain. Our SAW sensor includes Lithium Niobate ($LiNbO_3$) as a piezoelectric substrate base material, with Polyisobutylene (PIB) film used for absorbing(sensing) material and Aluminum IDT electrodes. We have expanded on the inbuilt application present in COMSOL and varied the design parameters like thickness of PIB layer, concentration of gas, shape of electrodes, etc. We carried our simulation in COMSOL Multiphysics 5.6. The resonant frequency was estimated, it decreased in the presence of gas. This reduction(shift) was used to determine the presence of gas and to find the sensitivity of the sensor.

Keywords – COMSOL Multiphysics, MEMS gas sensor, surface acoustic wave, piezoelectric, gas detection.

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1. Introduction

Today oil and Gas industries have grown wide scale, with huge market and demand in every field, which has given further boost to the industry. These are spread over 1000 acres and hectors of land, with the pipelines spreading from 100's to 1000's of kilometres. But, since most of these gases are hazardous and flammable, their networking, controlled distribution and management need to be thoroughly monitored to avoid any havocs and terrible damage and loss of life, environment, money and resources. So, sensing the leaks and fixing them on time is one of the important aspects of monitoring and management systems. The direct physical monitoring of these processes is too tedious, ineffective, requires a thousand of volunteers for even monitoring a small plant and detection of minute quantities(ppm) of gases becomes impossible. Hence usage of sensors remotely is important. There are different types of sensors which can be used ranging from few metres to micro and nano meters. Since the plant is huge and we need thousands of sensors at various locations, MEMS becomes important as it helps in making miniaturized sensors, in large quantities which can sense effectively.

Out of the numerous sensors available we have decided to study the Surface Acoustic Wave (SAW) gas sensor. The reason being they have simple design, inexpensive, high frequency range, less vibration, can record small frequency changes, can be remotely operated, easy for maintenance, can detect variety of gases, etc. The sensor also has a few drawbacks which include complicated electronic circuits.

As the name suggests, surface acoustic wave is a mechanical wave that travels through the surface of an elastic material(solid). The amplitude of the wave decreases exponentially with the depth of the material. The structure and working of the sensors have been explained in detail further in the report. We have referred largely to the paper by *Staline et al.* And report by *Arshpreet et al.* on SAW gas sensors and the inbuilt application library in COMSOL.

1.1. Motivation

We went through various research papers and literature for MEMS sensor, and read about various types of sensors. Then, we selected the SAW based gas sensor for detection of volatile gases like chloromethane, dichloromethane, chloroethylene, etc.

The major motivation for this project was to identify the various parameters related to SAW sensor, understand its geometry and design, to see its effectivity to varying conditions. In most of the research papers studies we found that simulations were caried out on basic design for various gases, but we didn't find much work on various geometric analysis, which motivated us further to study these aspects. Besides this, we also wanted to explore the SAW sensor in further detail for our understanding and understand it working more thoroughly.

These all aspects helped us to carry out simulation on the geometry and various gases to arrive at some results and conclusions which are discussed further thoroughly in the report.

1.2. Importance of the problem

Sensing the leaks and fixing them is an important challenge today in oil and gas industry. Earlier we have faced many major accidents like the Bhopal gas tragedy which had tremendous damage and loss of life and resources, along with everlasting effects which are also felt today in the surrounding areas. Besides these, earlier the gas and oil industry pipelines leakage issues were limited for the oil fields, transportation vehicles and industrial errors. But today with increasing no. of underground pipelines even for gas supply to homes (E.g., MNGL), it becomes necessary to effectively monitor the process.

Due to these reasons, we have tried to vary different parameters in order to increase the sensitivity of the sensor.

1.3. Aim, Objectives and Scope of the project

1) **Aim** – To study SAW MEMS based gas sensors for organic volatile gases, its working, to simulate the sensor with varying parameters and electrode shapes, and to understand its effect for various gases.

2) **Objective** – The main task of our project is to study the variation of thickness of Polyisobutylene (PIB) film, concentration of gases - Chloromethane (CM), Dichloromethane (DCM), Trichloromethane (TCM), and Carbon Tetrachloride (CT), shapes of electrodes, size of sensor, and temperature variation and compare the results.

3) **Scope** – This study will help us to design better MEMS sensor according to the application needed, to choose and geometry and parameters for effective detection.

2. Background and Literature review:

We have referred various papers and did a detailed study about SAW gas sensor in this paper and found out following details :

2.1. Structure of SAW gas sensor:

The structure of SAW based gas sensor consists of three main parts called substrate, interdigitated transducers and a sensing layer.

2.1.1. Substrate

It is the base of the device. It is generally made up of LiNbO3(Lithium Niobate), quartz, and other piezoelectric materials can be used.

2.1.2. Interdigitated Transducer (IDT)

The IDT are the components which transmits electrical signals to the device in the form of acoustic waves. The output waves is also measured and transmitted in the form of electrical signals by IDTs. This helps us in measuring the output frequency of the wave.We have used aluminium in this report as the material for IDT. The IDTs are usually given the shape of a comb to have more surface area exposed to the sensing layer. The performance parameter of the device can be altered by changing the shape, width or thickness of the IDT.
Tin (Sn), Gold (Au), Platinum (Pt), Palladium (Pd),etc. can also be used.

2.1.3. Sensing layer

The sensing layer is deposited between the IDT and on top of the substrate. These sensing layers selectively absorb gases to which they are exposed. This causes the change in the weight of the layer and thus changing the frequency of the wave propagating through it. ZnO(zinc oxide), PIB(Polyisobutylene), Palladium, etc. are some of the layers which can be used in this device. We have used the PIB layer while simulating and calculating the results.

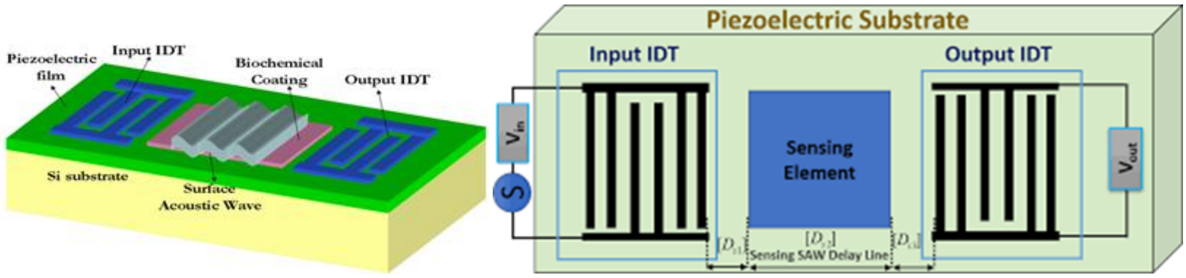

Figure 1: SAW sensor basic structure

2.2. Working Principle

Piezoelectric effect is used for detecting the gases. The gases leaked is sensed with the help of change in the frequency values. The electrical signals are converted into the surface acoustic waves by Interdigitated transducers. The alternating voltage is provided to the IDTs. The change in voltage causes the piezoelectric material to cause strains alternatively. These strains produced causes a wave to propagate along the material. This mechanical acoustic wave is then converted to electrical signals by the output IDT. The wave is propagated from input IDT to output IDT. Reverse piezoelectric effect is used while converting electric signals into acoustic wave.

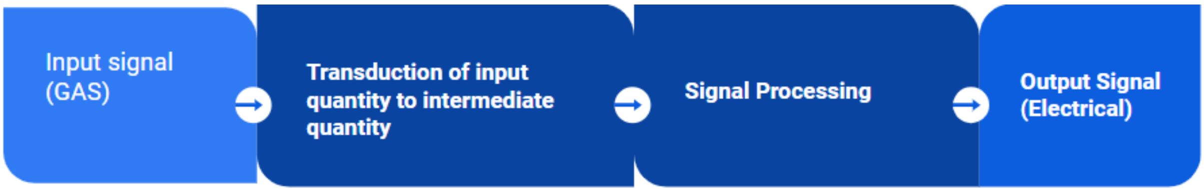

Figure 2: Basic Working of Gas Sensors

When the gas is selectively absorbed by the sensing layer the mass of the layer increases. The increase in mass changes the density of the layer. This change in density causes the change in the frequency of the acoustic wave generated. The output frequency is different from the original frequency. This frequency shift tells us about the leakage of the gas.
The concentration of the gas in air is measured using the following formula

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

Where P is the air pressure, R is the gas constant and T is the air temperature.
The partial density of the gas absorbed is calculated from the given equation.

$$\rho_{gas/PIB} = \mathrm{KMc} \quad \text{--------------(2)}$$

K is the air/PIB partition coefficient for the gas. C is the concentration of gas in air and M is the molar mass of gas.

$$\rho_{total} = \rho_{PIB} + \rho_{gas/PIB} \quad \text{---------------(3)}$$

The above density gives the total density of PIB layer (sensing layer).
The shift in the frequency due to change in the mass is obtained by using the formula

$$\frac{\Delta f_m}{f_0} = \frac{\Delta v_m}{v_0} = -\mathrm{K} f_0 h [\mathrm{K}_1(\rho) + \mathrm{K}_2(\rho) + \mathrm{K}_3\left(\rho - \frac{4\mu(\lambda+\mu)}{v_0^2(\lambda+2\mu)}\right) \quad \text{-------------(4)}$$

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, is the nominal saw velocity, λ and μ are Lame constants of the film. (Ref: 1)

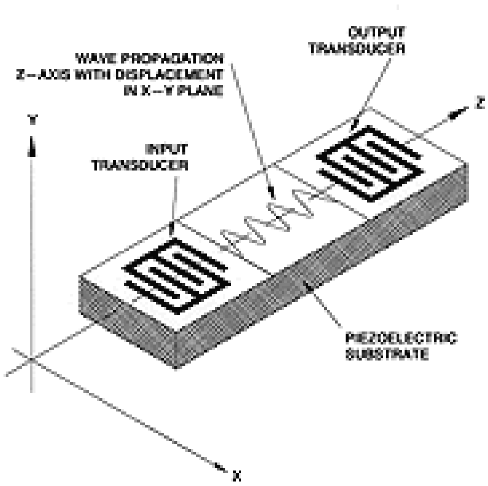

Figure 3: Propagation of wave on SAW sensor

(Ref. https://qtxasset.com/files/sensorsmag/nodes/2000/936/1000_68h.gif)

2.3. Various gas properties:

Gas	K[5]	M[5]	$\rho_{gas/PIB}$ (Kg/m³)
Chloromethane	0.5538	50.4	7.3589×10^{-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: Gas Properties

Various types of gases which are used in our simulation has the following properties:

CM: Chloromethane - (CH_3Cl): clear, colorless, odorless, flammable, sweet odor gas, highly toxic
Uses: Important industrial reagent; mostly not used in Consumer products; production of silicone and polymers; used in Petroleum refining, used as methylating and chlorinating agent in organic industry; foam-blowing agent, pesticide and fumigant
Hazards: it affects breathing level, long time exposure may damage testes, its contact can cause frostbite, severe skin and eye burns, higher levels can cause dizziness, drowsiness, unconsciousness, convulsions, and death, blurred vision and brain damage.

DCM: Dichloromethane – (CH_2Cl_2): clear, colorless liquid with a slightly sweet scent
Uses: used as a solvent in potent paint strippers/ paint thinner, as a propellant in aerosols, in the manufacture of photographic film, and as a process and industrial solvent in the manufacturing of drugs.
Hazards: It can cause damage to brain and Central Nervous System (CNS). The EPA classifies it as carcinogenic since its high exposure causes lung and liver cancer. It also causes harm to skin, eyes, liver and heart. It also leads to dizziness, drowsiness, numbness and tingling limbs, and nausea. Severe effects can be loss of Consciousness and death.

TCM: Trichloromethane - ($CHCl_3$): colorless, strong smelling volatile liquid with sweet odor, non-combustible, low solubility in water.
Uses: it is used as anesthetic during surgery; solvent in industry for iodine, alkaloids, fats; manufacturing of various industries; etc.
Hazards: Its severe use ca cause damage to nervous system, liver and kidneys and severe effects can lead to death.

CT: Carbon Tetrachloride - (CCL_4): colorless, sweet smell liquid, non-flammable

Uses: used for producing refrigerants and propellants for aerosol; solvents for oils, fats, lacquer, varnishes, rubber, waxes, resins; grain fumigant; dry cleaning agent, fire extinguisher, degreasing agent, spot remover, insecticide
Hazards: its vapor can affect CNS, degenerate the liver and kidneys, cancer, long exposure may lead to coma and death.

2.4. Simulation

As we can see the pattern of IDT is repeated over the layer. For simplicity in simulations, we have used a 2-D model cross section as shown in the fig. 4

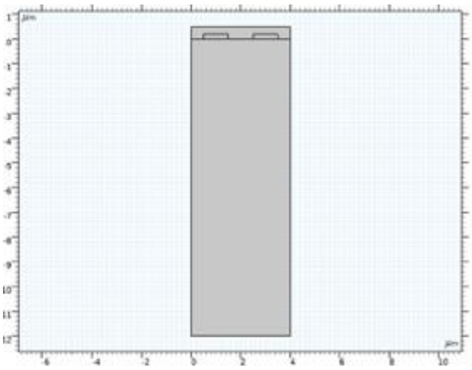

Figure 4(a): 2-D model used for simulation.

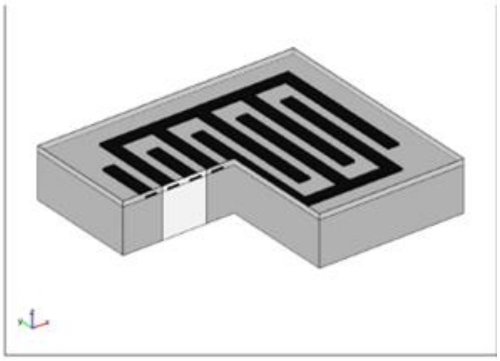

Figure 4(b): Saw based sensor 3-D model

2.5. Techniques for fabrication

The fabrication process is started with the standard techniques required for manufacturing MEMS device. Thermal evaporation, photolithography, sputtering and chemical etching are some of the major steps followed by the standard techniques.

The initial step starts with the sample cleaning, followed by substrate metallization, Photolithography, etching and finally with deposition of layers.

2.5.1. Sample Cleaning

The class 1000 or more clean room facility should be used for the cleaning process. The Lithium Niobate substrate of the required dimensions has to be rinsed with Trichloroethylene. The substrate is then ultrasonicated for about 30 mins in acetone. The sample is then rinsed for 5 minutes with Isopropyl Alcohol. Now the sample is wet, we need to make it dry. So, the compressed nitrogen gas is blown over it.

2.5.2. Substrate Metallization

The parameters that are used for deposition are the current of 20 Ampere, Pressure of 5.1 E-6 torr, time taken and thickness of the layer were also taken into consideration. The further step is to cut the wafer into smaller rectangular shapes.

2.5.3. Photolithography

The Interdigitated transducers design patterns are made using photolithographic masks. This is done over the substrate previously made. The high-resolution printer is then used to design and fabricate the masks over thick films of PMMA (Polymethyl methacrylate). The process of photolithography was carried out by using a negative or positive photoresist. The Positive or negative photoresist can be used based on the conveniency. The mask is held over the substrate sample and exposed to almost perpendicular UV rays. These rays help to make the photoresist more or less soluble in the chemicals. The design on the mask is transferred onto the metal layer on the substrate. The temperature and humidity is maintained within a particular range.

The positive photoresist is the one which becomes soluble when exposed to UV light. The vice versa is the negative photoresist which becomes insoluble when exposed to UV light. The deposition of the photoresist is done by using a spin coater. Parameters such as spin speed, time, and thickness are taken into consideration while this deposition.

The sample is soft baked after the photoresist coating. Soft baking is the process in which the sample is heated to around 75 C for 25 minutes. This is done using a hot plate. This is done to harden the photoresist. This hardened film is then exposed to UV light. The wavelength and exposure time parameters are taken into consideration for different photoresists. The KOH solution is used as a developer to develop the sample. The sample is developed for about 7-8 seconds. Then it is washed with Deionised water to remove any developer solution which sticks to the sample.

2.5.4. Chemical Etching

The metallised regions which are not required are then removed by wet etching. The photoresist protects the required material. The timing of this etching process is critical. The stronger or weaker (over or under) etching may lead to different dimensions than the design. This effect can distort the electrical characteristics of the device and can hamper the application as well.

Two different ways can be used for etching the sample. Heating the etchant to 45 C and immersing the sample into the etchant is the one of the ways. Here, The the etchant contains 8:5:5 ratio of H_3PO_4, HNO_3 and DI water. The formation of bubbles is prevented by constant stirring. The bubbles cause problems such as regressing the etching and some under etched parts may be found. The second way of etching is to use diluted KOH. Even the etching and aluminium is done without stirring. To etch a layer of about 200nm, 2-3 minutes of time period is required.

2.5.5. Deposition of sensing layer

PIB layer is deposited using the sol-gel method. The parameters required for deposition are Speed of coating, molarity, temperature and time required.

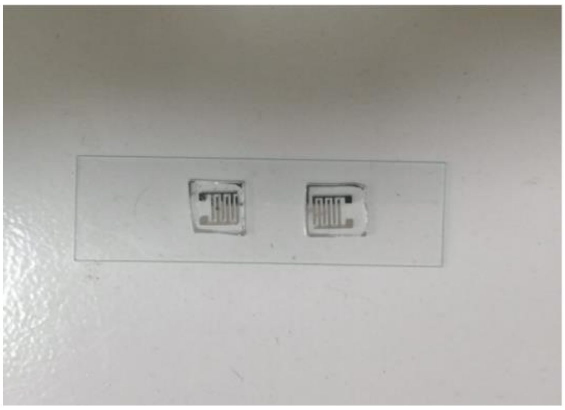

Fig 5: Fabricated SAW sensor. (Ref: 3)

3. Project Discussion (simulation details)

The simulation was carried COMSOL Multiphysics 5.6. The MEMS Module of COMSOL allows efficient and easy modelling of saw gas sensors. This module couples the solid mechanics and electrostatics equations and solves them simultaneously to predict various results discussed in the report below.
The model of SAW gas sensor is already present in application library of COMSOL. We have expanded our project on this model. Since the stresses generated by the waves are planar and negligible in third dimension, we have done 2D or Planar simulation.

3.1. Parameters

The model was parameterized in order so that we can change the input and geometry of the SAW gas sensor easily.
The Parameters are as follows,

Name	Expression	Value	Description
p	1[atm]	1.0133E5 Pa	Air pressure
T	25[degC]	298.15 K	Air temperature
c0	100	100	DCM Concentration in ppm
c_DCM_air	1e-6*c0*p/(R_const*T)	0.0040874 mol/m³	DCM concentration in air
M_DCM	84.93[g/mol]	0.08493 kg/mol	Molar mass of DCM
K	10^1.4821	30.346	PIB/air partition constant for DCM
rho_DCM_PIB	K*M_DCM*c_DCM_air	0.010534 kg/m³	Mass concentration of DCM in PIB
rho_PIB	0.918[g/cm^3]	918 kg/m³	Density of PIB
E_PIB	10[GPa]	1E10 Pa	Young's modulus of PIB
nu_PIB	0.48	0.48	Poisson's ratio of PIB
eps_PIB	2.2	2.2	Relative permittivity of PIB
switch	0	0	Switch for adding DCM density
vR	3488[m/s]	3488 m/s	Rayleigh wave velocity

width	4[um]	4E−6 m	Width of unit cell
f0	vR/width	8.72E8 1/s	Estimated SAW frequency
t_PIB	0.5[um]	5E−7 m	PIB thickness

Table 2: SAW sensor for gas parameters

We have varied the parameters concentration of the gas(c0), thickness of PIB(t_PIB) and properties related to DCM as the gas that needs to be detected changes.
Instead of defining these values at each stage of the modelling, if parameters are mentioned then we need to change the value only once to change it everywhere in the simulation. This saves times and makes simulation easier.

3.2. Geometry

We have designed the geometry in COMSOL itself. As mentioned earlier the simulation is planar hence this is a planar geometry. As mentioned earlier we have tried to vary the dimensions and shapes of the electrodes present in the geometry.

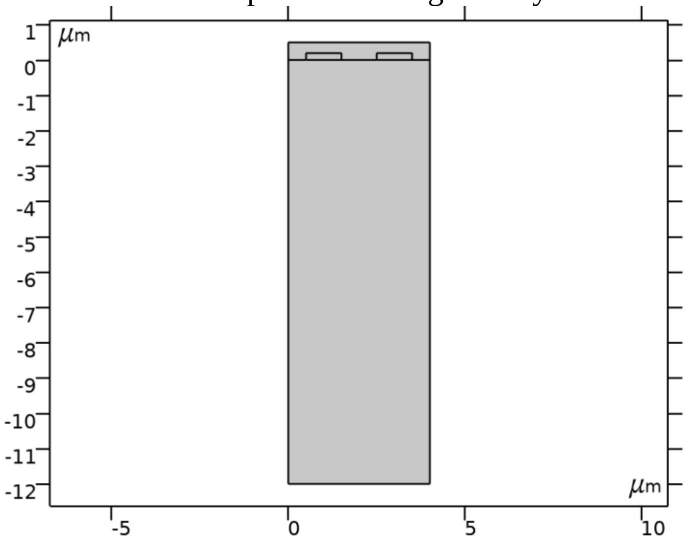

Figure 6: Basic Geometry

The thickness of the is given as t_PIB and the dimensions of the electrodes (= width/4× 0.4*t_PIB) and the height(=3*width+t_PIB) are given in terms of the width and PIB thickness. So, when width and thickness are varied the rest of the geometry also varies accordingly.

Shapes of electrodes:

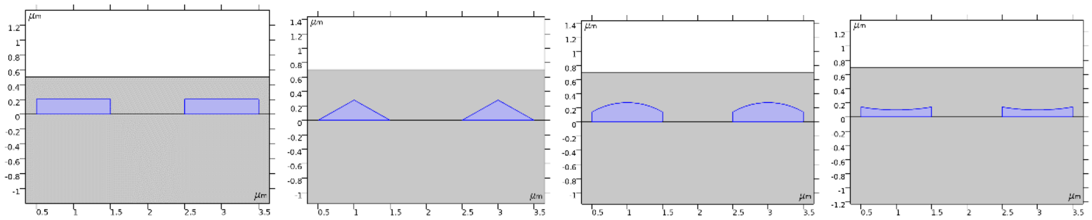

Figure 7: Different shapes of electrodes

These 4 shapes of electrodes were used which were rectangular, triangular, outward curved and inward curved.

3.3. Materials

Three different materials are required in SAW gas sensor. All the geometries have used the same materials which are Aluminium for electrodes, PIB (Polyisobutylene) as a sensing film and Lithium Niobate ($LiNbO_3$) which is the piezoelectric substrate.

The allocation of materials is as follows:

1. $LiNbO_3$

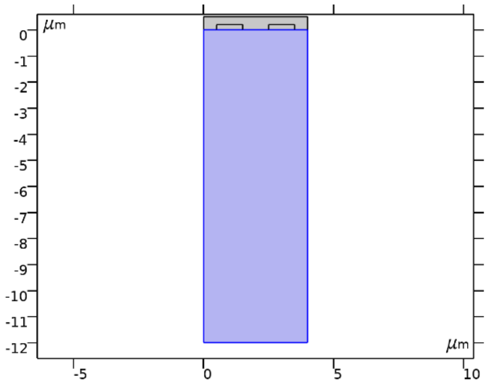

Figure 8(a): Piezoelectric base : $LiNbO_3$

2. PIB

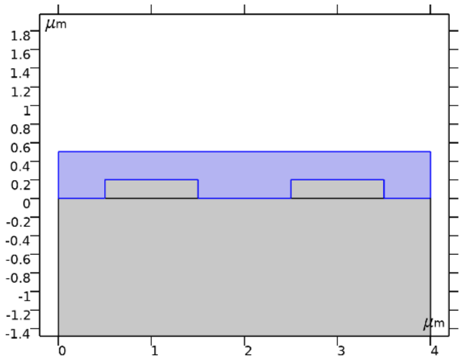

Figure 8(b): Sensing Layer : PIB

3. Aluminium

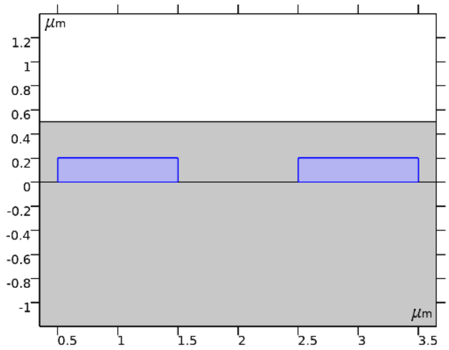

Figure 8(c): IDT Electrodes : Aluminium

3.4. Governing equations and Boundary Conditions

3.4.1. Governing Equations-

The solid mechanics and electrostatics equations were solved simultaneously by COMSOL to obtain the desired result. The Multiphysics in COMSOL takes care of the piezoelectric effect and has a different domain than solid mechanics and electrostatics.

1. Solid Mechanics

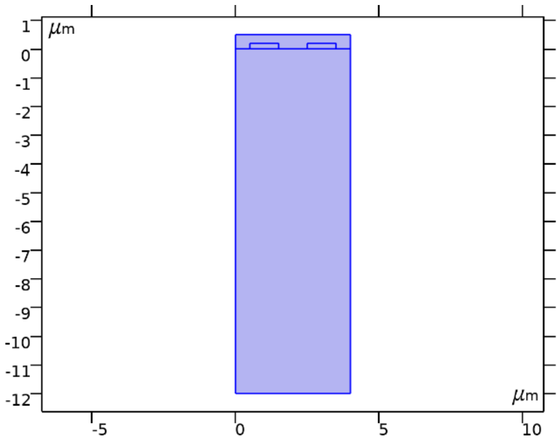

Figure 9(a): Solid Mechanics

EQUATIONS

$$-\rho\omega^2\mathbf{u} = \nabla \cdot S, \quad -i\omega = \lambda$$

2. Electrostatics

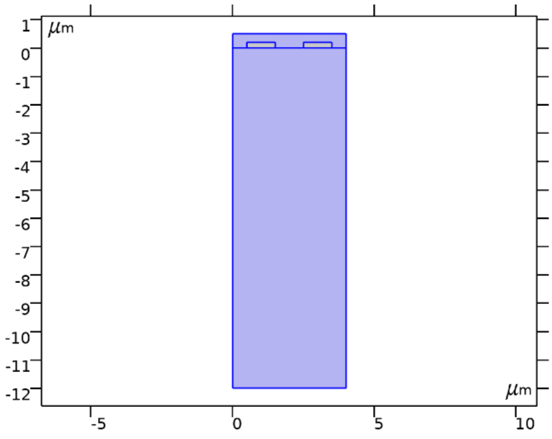

Figure 9(b): Electrostatics

The electrodes were excluded.

EQUATIONS

$$\nabla \cdot \mathbf{D} = \rho_V$$

$$\mathbf{E} = -\nabla V$$

3. Piezoelectric effect

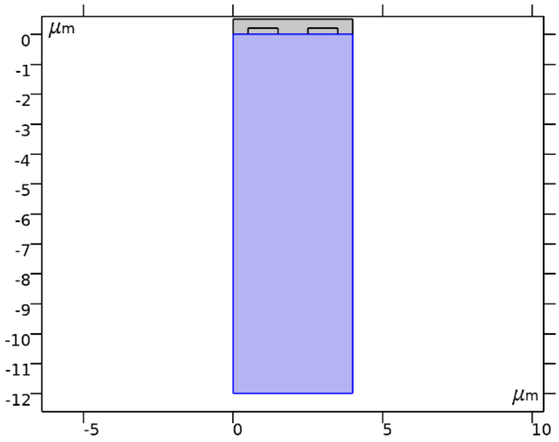

Figure 9(c): Piezoelectric effect

Only lithium Niobate domain was chosen.

3.4.2. Boundary conditions –

The initial values were taken as 0.

1. Fixed constraint

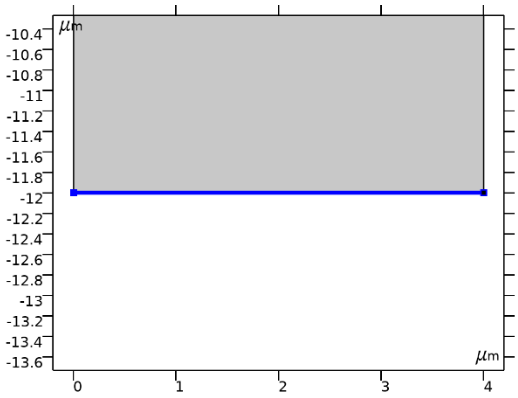

Figure 10(a): Fixed Constraint

2. Free

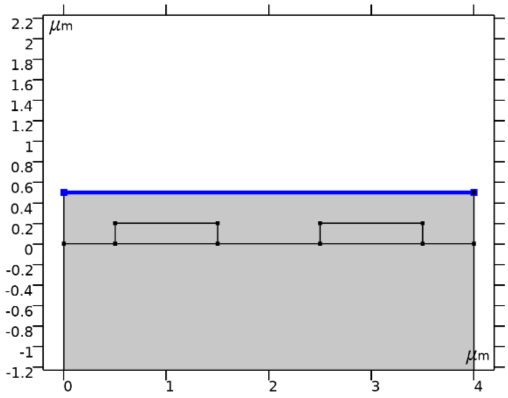

Figure 10(b): Free Condition

3. Periodic Condition

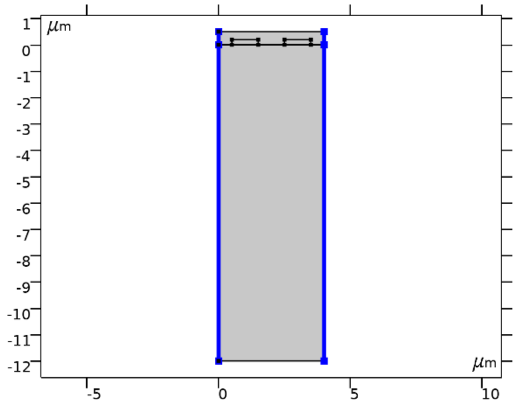

Figure 10(c): Periodic Condition

As mentioned earlier this model is one unit of the entire sensor. This condition allows us to define from where the unit starts and ends. We can do this because of the periodic symmetry of the sensor. This condition is applied both in solid mechanics and electrostatics.

4. Charge conservation

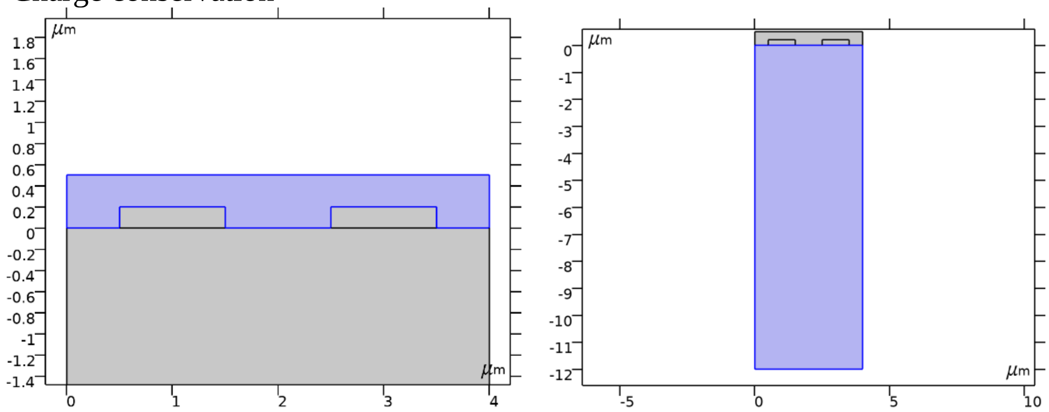

Figure 10(d): Charge Conservation

COMSOL provides this condition in order to get accurate results when different types of insulations(dielectrics) are present next to each other. In this case PIB and Lithium Niobate.

5. Zero charge

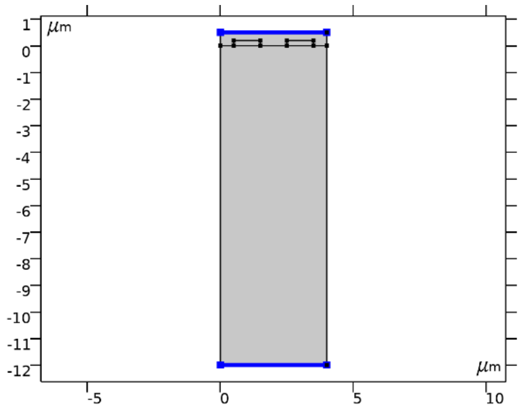

Figure 10(e): Zero charge

This condition by default defines the exterior boundaries of the model and that electric potential is discontinuous across it.

6. Ground and Floating potential

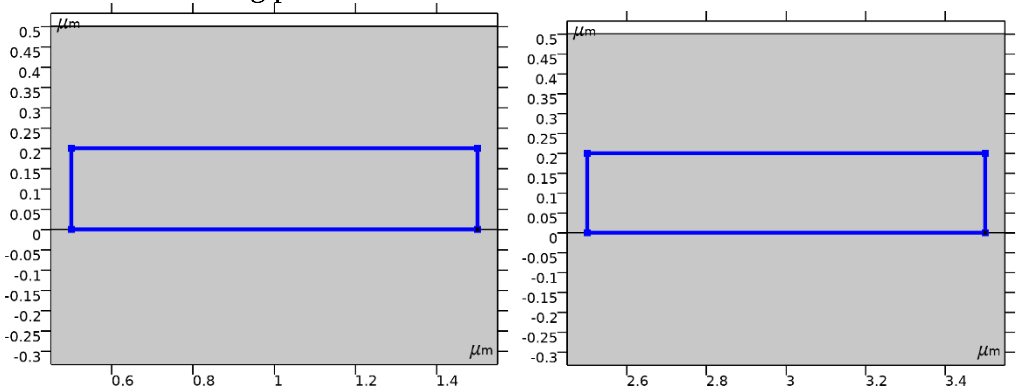

Figure 10(f): Ground and Floating potential

The left electrode is grounded and the right one is given floating potential as shown above. These conditions give us the surface of the conductor. In this case aluminium electrodes.

3.5. Mesh and Study

3.5.1 Mesh-

The meshed geometry is as follows,

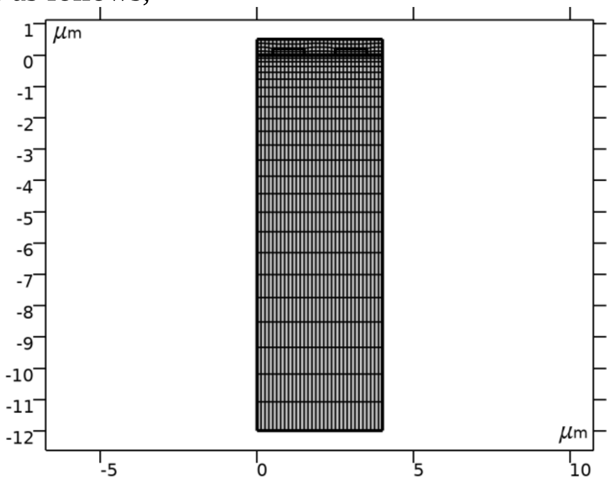

Figure 11: Mesh

Edge type meshing was done for the model. Free quad was used near the electrode boundaries so that unstructured quadrilaterals could be formed to mesh properly.

3.5.2 Study-

Parametric sweep was used in order to vary-

1. The PIB density when gas is absorbed and when gas is not using the parameter switch ([0 1])
2. Concentration of the gas using parameter c0 ([80:10:120])
3. Thickness of PIB using the parameter t_PIB ([0.3:0.05:0.7])

Eigenfrequency study as performed in order to find the natural frequencies of the senor. As mentioned earlier the frequency f0 was found out using the Rayleigh velocity. This f0 is the estimated natural frequency of the sensor. So we will be finding only the frequencies near this f0 which saves the computation time.

4. Results and discussions

The simulation was carried out and various results were plotted.

4.1. Resonance -

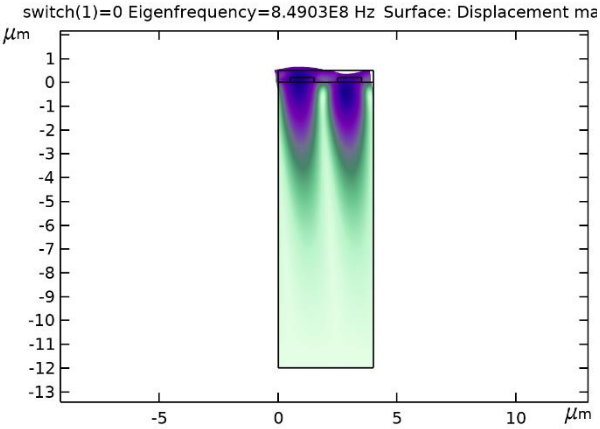

Figure 12(a): Resonance Mode Shape

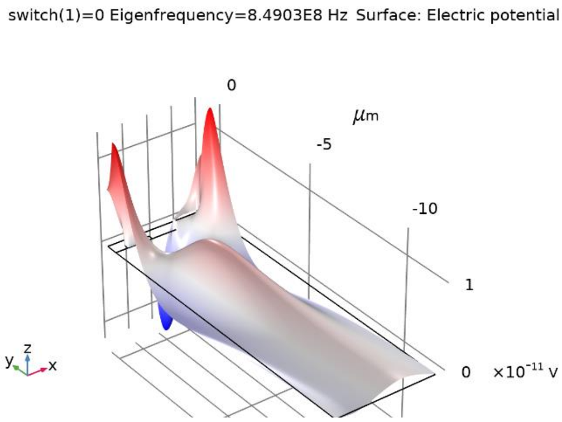

Figure 12(b): Resonance Electric Potential

The figure on the left shows resonant saw mode with frequency of 8.4902524790860 99E8 Hz. This mode occurs due to constructive interference of propagating waves. As discussed earlier, the waves occur at the surface and the amplitude dies as the depth increases. The figure on the right shows the electric potential distribution and deformation and is symmetric.

4.2. Anti-resonance-

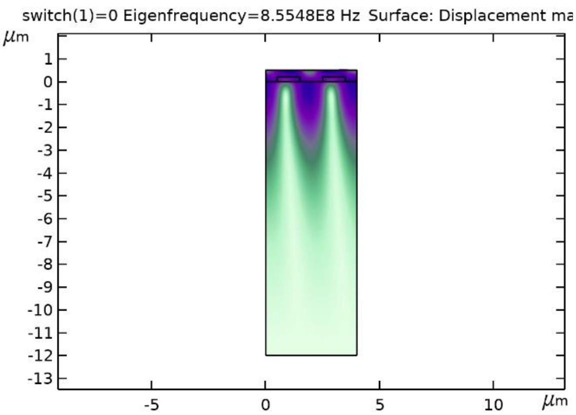

Figure 12(c): Anti-Resonance Mode Shape

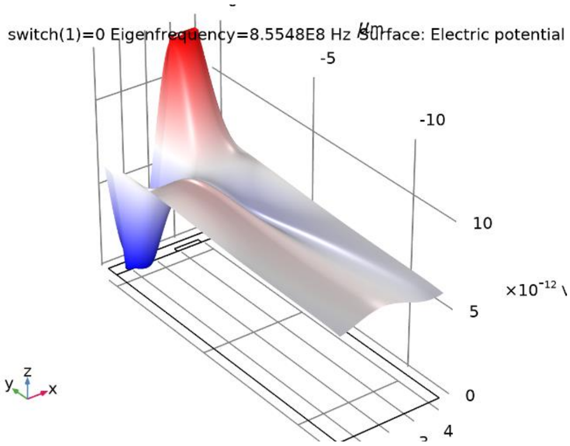

Figure 12(d): Anti-Resonance Electric Potential

The figure on the left shows anti-resonant saw mode with frequency of 8.554837939739076E8 Hz. This mode occurs due to destructive interference of propagating waves. The figure on the right shows the electric potential distribution and deformation and is anti-symmetric.

By comparing different gases, we can conclude that the frequency shift for the gases decreases in the order Carbon Tetrachloride, TCM, DCM, and CM.

4.3. Variation of Different Parameters

4.3.1. Thickness

- As thickness of PIB layer increase, we get better frequency shift (can be detected easily).
- These 4 gases (DCM, CM, TCM, and CT) lie in different frequency ranges so we can detect these gases based on the frequency shift value for a particular concentration (100 ppm here).
- Change in Frequency varies almost linearly for DCM, CM and TCM but there is a change in slope for Carbon Tetrachloride
- Carbon Tetrachloride can be detected easily after 0.35um thickness of PIB.

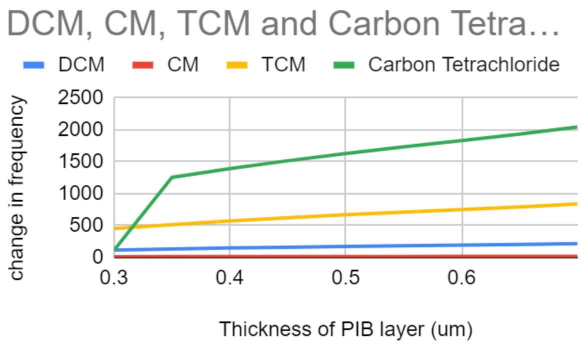

Figure 13(a): Thickness of PIB film

4.3.2. Concentration

- Linear variation of frequency shift with change in concentration for all the gases.
- We cannot conclude the correct gas and its concentration if there are multiple gases as the frequency shift can overlap with other gases for different concentrations.
- Approximate prediction of concentration of gas for a frequency change is possible if we know the gas.

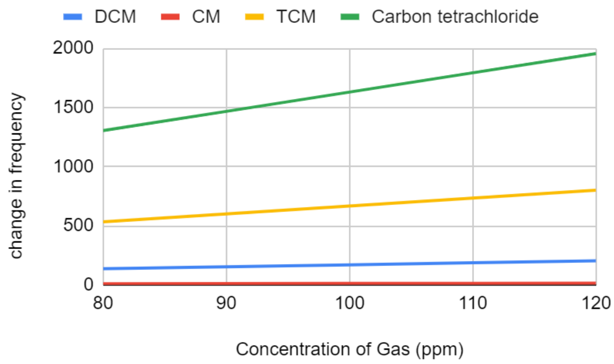

Figure 13(b): Concentration of gas

4.3.3. Sensitivity

- *Sensitivity is defined as ratio of resonant Frequency shift to partial density of gas absorbed by PIB layer (sensing film).*
- There is linear variation of sensitivity with concentration and does not change much with the type of gas in this case.

- Even though the frequency shift of CM is less compared to other gases, its density is very low due to which the sensitivity is as high as other gases. Thus the SAW sensor is equally sensible to CM as it is sensible to other gases.

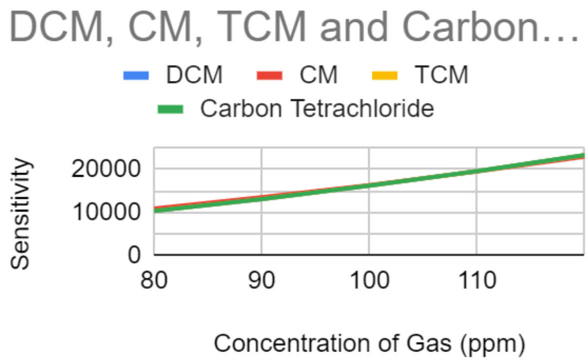

Figure 13(c): Sensitivity

4.3.4. Temperature

- The change in Frequency shift is not significant with change in Temperature.
- The frequency change is not affected to a large extent even after a change of 30 ^{o}C.
- The same conclusion can be drawn even for different temperatures with respect to concentration, sensitivity, Thickness of PIB film as discussed above.
- The frequency shift decreases with rise in temperature.
- The frequency shift is affected by almost 2% for every 5 C rise in temperature.

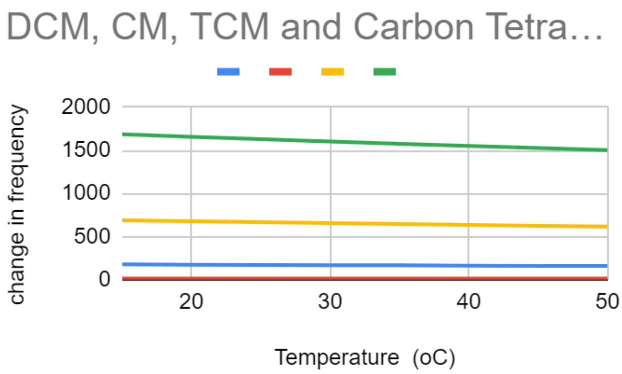

Figure 13(d): Temperature

4.3.5. Width

- The change in frequency is increases if we decrease the width considered for unit cell.
- This sensitivity also follows the same trend for decrease in width. So, the gas is more detectable for lesser width.

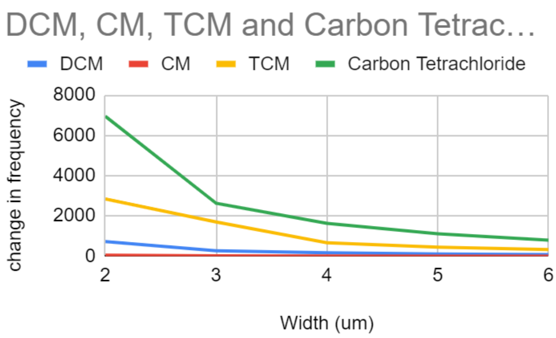

Figure 13(e): Width of unit cell

4.4. Shapes of Electrodes

Resonance and Anti-Resonance Frequencies.

4.4.1. Thickness

- Frequency shift for rectangular electrode is less as compared to other shapes.
- The maximum shift in frequency for all the shapes is around 0.6um thickness of PIB. So we can take the thickness of PIB film around 0.6 um for better results and easier detection.

4.4.2. Concentration

- Frequency shift is more for inside curved electrode at all concentrations
- The change in frequency decreases in the order of inside curved, triangular, outside curved and rectangular shaped electrode.

4.4.3. Sensitivity

- The sensitivity increases with concentration of gas.
- When compared with different shapes the same order is followed for frequency shift as of the concentration.

We can see a considerable change in frequency with change in shape in resonance mode. But the change in frequency for all the shapes is almost the same for anti-resonance mode.

Resonance

<u>Thickness of PIB film</u>

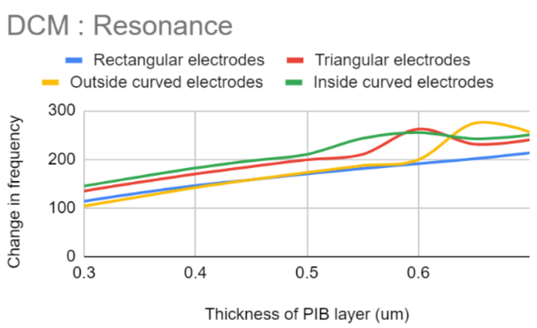

Figure 14(a): Thickness of PIB film

<u>Concentration of DCM</u>

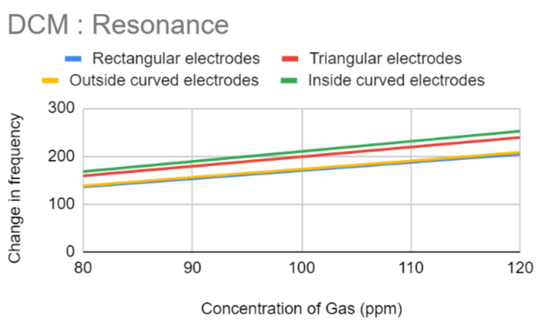

Figure 14(b): Concentration of gas

<u>Sensitivity</u>

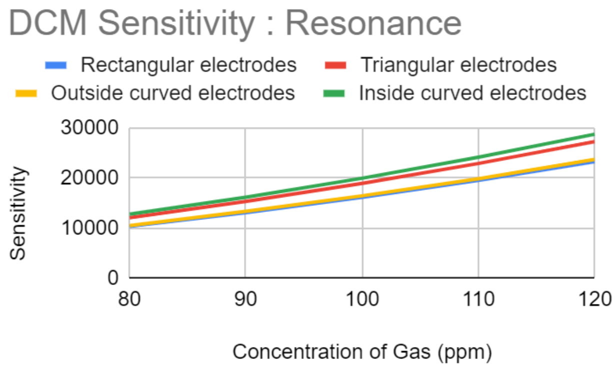

Figure 14(c): Sensitivity

Anti-Resonance

<u>Thickness of PIB film</u>

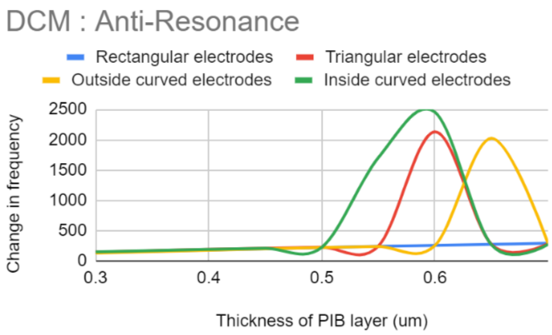

Figure 15(a): Thickness of PIB film

<u>Concentration of DCM</u>

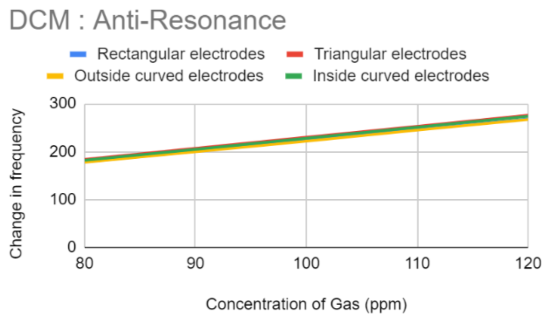

Figure 15(b): Concentration of gas

<u>Sensitivity</u>

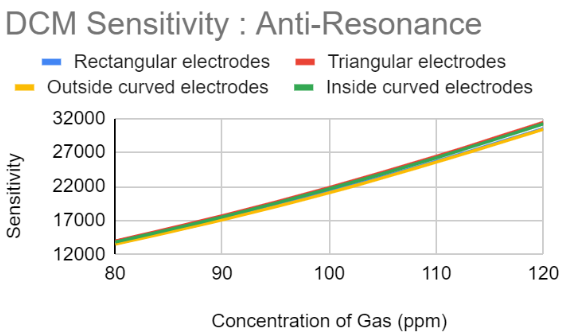

Figure 15(c): Sensitivity

Excel Sheets with all values and Calculation

For 4 gases Comparison: https://docs.google.com/spreadsheets/d/1b9tdsC-5RE5N_iz5n-SKpZcorUgzRAWfY8j-E58cDYc/edit?usp=sharing

For shapes of electrodes: https://docs.google.com/spreadsheets/d/1yEM5WTEsyzfb-W1mfdqKvI2AAf9F91OgoJY8zL9SJ9g/edit?usp=sharing

5. Conclusion

In present work, we carried out variation of different shapes of electrodes, and also varies the gases for rectangular electrodes.
From this study, we have following conclusions:

- Thickness of PIB film > 0.5 um (for large shift in frequencies)
- Non-conventional electrode shapes like curved and triangular electrodes give more frequency shift compared to conventional rectangular electrodes. So, we should try more shapes of electrodes for better changes along with keeping the manufacturing capabilities in mind.
- Frequency shift increases with decrease in width, but decreasing width to large extent can make manufacturing difficult.
- SAW Sensor can work effectively at all room temperatures with hardly any change in frequency shift. These sensors give more shifts at lower temperature.
- Sensitivity for all the gases is same irrespective of their concentration and frequency shift, hence they can detect all the gases effectively.
- Even though CM, DCM, TCM and CT belong to same family and almost similar properties, they give different frequency changes for different concentration. Therefore, this sensor can be used for detection of various gases which may belong to same family.

6. Directions for Future Work

The SAW gas sensor is a vast topic and unexplored topic. Future work is as follows,

- Simulation of results for different gases at different concentration.
- To study the stress developed at the interface of PIB and piezoelectric substrate in order to see if sensor works at operating frequency without any damage.
- We can also use various other materials for piezo base, electrodes and sensing film, and thus try to choose the best materials.
- This study doesn't focus on manufacturing methods for various electrode shapes, its fabrication can be thoroughly studied.

7. Bibliography and References

[1] Staline Johnson, Dr. T. Shanmuganantham. Design and Analysis of SAW Based MEMS Gas Sensor for the Detection of Volatile Organic Gases. International Journal of Engineering Research and Applications, Vol.1 4, Issue 3(Version 1), pp 254-258.

[2] K. Srinivasa Rao, A. Haumaiah and P. Sri Sairam. Design and analysis of saw gas sensor. European Journal of Applied Engineering and Scientific Research, 2012, 1(2), pp 37-42.

[3] Singh, Arshpreet. “Design and Simulation of Saw Based Gas Sensor.” Thapar University, 2017.