A
Thesis Report
On

“Design and Simulation of Saw based Gas Sensor”

Submitted towards the fulfilment of requirement for the award of degree of

Master of Technology
In
VLSI Desgin

Submitted By:
Arshpreet Singh
Roll No: 601562004

Under the Supervision of
Dr.Anil Arora
Assistant Professor

ELECTRONICS AND COMMUNICATION ENGINEERING DEPARTMENT
THAPAR UNIVERSITY
(Established under the section 3 of UGC Act, 1956)
PATIALA – 147004 (PUNJAB)
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DECLARATION

I, Arshpreet Singh, hereby declare that the work presented in this thesis entitled **"Design and Simulation of SAW based Gas Sensor"** in partial fulfillment of the requirement for the award of degree of Master of Technology in VLSI Design submitted at Electronics and Communication Engineering Department, Thapar University, Patiala is an authentic record of work carried out under supervision of **Dr. Anil Arora** (Assistant Professor, ECED, Thapar University) from January 2016 to July 2017. The matter presented in this has not been submitted either in part or full to any other university or institute for the award of any other degree.

Date: 18-8-17
Place: Patiala

Arshpreet Singh
601562004

It is certified that the above statement made by the student is correct to the best of my knowledge and belief.

Date: 18 Aug. 2017
Place: Patiala

Dr. Anil Arora
Assistant Professor, ECED
Thapar University, Patiala

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ABSTRACT

There has been a great interest in Surface Acoustic Wave (SAW) based gas sensors in recent years. SAW based gas sensors can efficiently detect the change in mass, modulus and conductivity of the sensing layer due to the adsorption of gas over the surface. Piezoelectric effect is used as the working principle in the operation of SAW based gas sensors. The advantages of SAW based gas sensors include small size, robustness, low cost, high sensitivity, portability and high accuracy.

In the present thesis work, different geometries of SAW based gas sensors are studied, designed and simulated for sensing hydrogen (H_2) gas. COMSOL Multiphysics software is used to design and simulate the proposed models of the gas sensor. Different parameter selections, boundary conditions, study settings etc are identified and optimised from the outcomes of the study based on literature review. Various design parameters of the gas sensor are optimized. The electrode thickness is optimized to 200nm and electrode material is selected as aluminium as per simulation results optimizations. The thickness of intermediate layer is optimized to be 0.6 μm, with maximum displacement shown by the gas sensor and hence the sensing results. The thesis is concluded with few fabrication steps that are performed in the laboratory.

TABLE OF CONTENTS

Chapter 5 Results and Discussions

LIST OF FIGURES

LIST OF TABLES

Page No

CHAPTER 1

INTRODUCTION

This chapter presents a basic introduction to gas sensors and SAW devices. Various aspects and working of SAW based gas sensor is also presented. Further a brief overview of some hazardous gases is given. In the end of the chapter thesis organization is also present.

1.1 Sensors

Smart sensors are very important in many fields of industry, control systems, biomedical applications, etc. Swift advancements in integrated circuit (IC) technologies have ushered new opportunities in the physical design of integrated sensors and Micro-Electrical-Mechanical Systems (MEMS). MEMS provide novel ways of merging sensing, signal processing and actuation on a microscopic scale. This lets both traditional and new sensors to be obtained for a large number of applications and operational environments. Basically a sensor is a device which receives an input signal or stimulus and produces a response. This device could convert the received signal into electrical form as sensing signal which could be used in electronic devices. A good workable definition of a sensor is a device that lets the transduction of chemical and physical properties at an interface into usable information. An ideal chemical sensor is a cheap, portable, reliable device that responds with precise and prompt selectivity to a specific chemical substance [1]. Thus a chemical sensor is a device that produces an electrical signal that is a function of chemical identity and/or concentration. Chemical sensors have the potential to be utilized in both fundamental studies of interfaces and the detection and measurements of chemical species.

Unfortunately, due to the broad spectrum of concentrations (many orders of magnitude) and substances which are encountered in real life, it’s impossible to attain this using a single technology. Out of necessity, one has to adjust the sensing systems to the sensing needs. The method used for chemical sensing can be divided into wide categories like;

1. Thermal sensors (that uses the energy generated through direct contact with an analyte)
2. Mass sensors (that detect alterations in mass loading due to the analyte),
3. Electrochemical sensors (that detect alteration in electrical properties)
4. Optical sensors (that detect alterations in spectra of light) [2].

Sensors are characterized in different ways such as measure of the magnitude of output signal generated as a response to an input quantity is called its sensitivity, its resolution is a measure of the smallest change of input quantity which it could detect and its selectivity is a measure of extent to which it could differentiate one input quantity from another. The following list gives both constraints and requirements for any sensor: repeatability, quick response, robustness, small size, ease of fabrication, temperature stability, etc.

1.2 MEMS

MEMS stand for Micro electro mechanical systems. It is the amalgamation of both electrical as well as mechanical components. It includes the components of very small dimensions usually of micrometres or millimetres dimension. At microscopic level, various sensors like thermal sensors, gas sensors or pressure sensors can be designed. MEMS components are fabricated by micro machining processes.

MEMS consist of wide variety of materials which can be utilized according to the application intended for. These materials include silicon, quartz, polymers, metals etc [3]. MEMS basically consists of four components as shown below

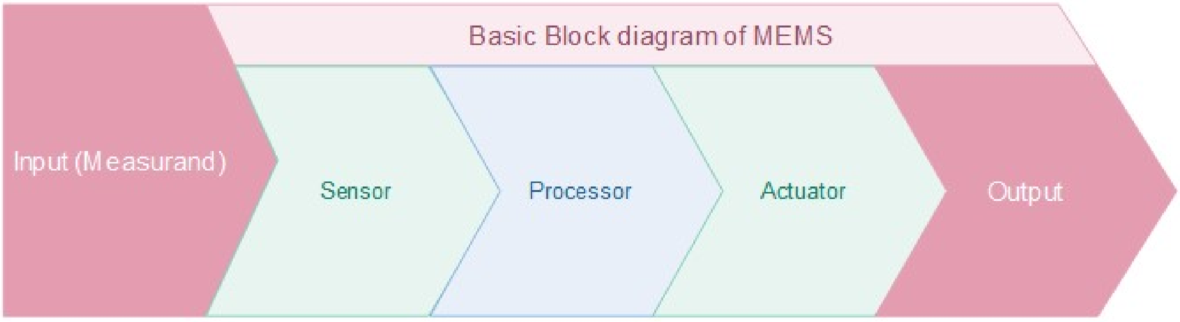


Fig 1.1 Basic flow diagram of MEMS

- Input signal: Input signal is the basic signal that we gave as input for processing. It can be of any form present in the environment.
- Sensor: Next is the sensor, which senses the input signal and converts in to electrical form if it is in non-electrical form.
- Processor: Processor does the processing by applying all the logical functions for the needed application.
- Actuator: Actuator does the reverse operation of sensor by converting the non-electrical form of energy in to electrical form of energy.

For fabrication of MEMS, there are three fundamental steps- Deposition, Lithography and Etching. In deposition, thin films of the suitable material are deposited on the substrate. There are two major methods which are used for deposition.

- Chemical reaction method
- Physical reaction method

Chemical reaction methods include chemical vapour deposition and thermal oxidation whereas physical reaction methods include physical vapour deposition (PVD) and casting.

Lithography is basically printing the patterns and transferring designs of IDT onto the metal layer on the substrate. Various lithography techniques are used in MEMS namely: photolithography, e-beam lithography, X-ray lithography etc.

Etching is removing the unwanted material from the substrate. It could be done in two ways namely dry etching and wet etching. When liquid chemicals are used for removing the materials from the samples, it is called wet etching while when materials are removed using bombardment of high energy ions, it is called dry etching.

1.2.1 Advantages of MEMS

1) Compatibility with IC leading to high performance
2) Batch fabrication
3) Small size and sturdiness
4) Lower cost of production
5) Low power consumption

1.3 Gas sensors

In most homes, appliances like gas furnace, water heater, boiler, cooking gas or other fuel burning devices produce combustion gases. Normally, these combustion products, which could include both noticeable smoke and various invisible gases, should be released to the exterior. Unfortunately, these might escape into the user dwelling environment instead, where these could raise different health and other concerns. Human senses can hardly detect these toxic elements of combustion gases, therefore sensors are needed to detect these when a certain gas concentration is present in atmosphere around us. Gas sensors can detect the presence of the harmful gases in the surrounding atmosphere. When the sensor interacts with the gas present around it, the properties of the sensor changes which reflects the sensing mechanism. One of the very popular technologies for making gas sensors is MEMS. This is mainly due of its minimal power consumption, sturdiness and very small size. Environmental conditions are deteriorating day by day. Among various gases, oxygen is vital and should be kept at adequate level while other hazardous gases should be controlled in order to maintain a healthy life. There are various types of sensors, among which surface acoustic wave (SAW) gas sensors are very popular as they have simple structure, long life time and robust nature [4]. Basic concept for a gas sensor is given in the figure below:

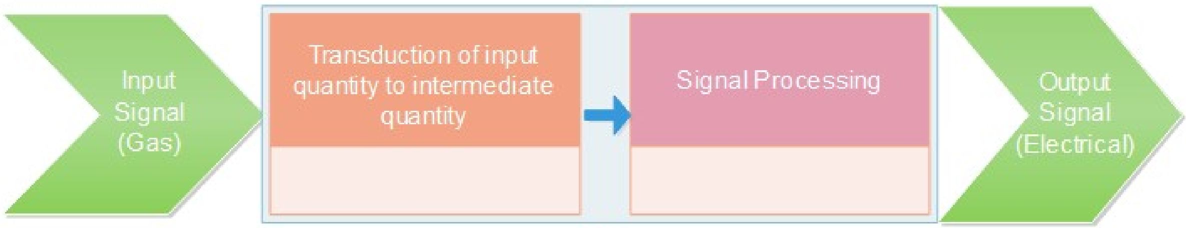


Fig 1.2 Basic concept for Gas sensor

Sensor device constitute two basic functions:

1) To sense the gas in its vicinity and
2) Signal translating mechanism that will translate the effects seen in the sensor to the corresponding measurable signals.

Gas sensing is done through the interaction of chemical species with the sensing surface. Chemical species which reacts with the sensing layer are absorbed on the layer and changes the properties of the sensing surface. Sensitivity of the layer towards a particular gas is of a major concern.

1.3.1 Applications of gas sensors

- Environmental monitoring
- Home safety
- Automobiles ventilation control
- Fire detection
- Leak detection
- Explosive gas detectors

1.4 Piezoelectricity

Piezoelectricity is basically a property of certain materials which allows them the conversion of mechanical energy into electrical energy and also electrical energy back to mechanical energy. The former is called piezoelectric effect and the latter is called inverse piezoelectric effect and the materials having this property to produce piezoelectric effect are called piezoelectric materials [5].

When a mechanical stress or strain is applied to a piezoelectric material, an electric charge is produced. Demonstration of this was done by Curie brothers in 1880.The converse piezoelectric effect was deduced by Gabriel Lippmann in 1881, which states that when an electric signal is applied to a piezoelectric material, the material gets strained [6].

The equations which govern the propagation of acoustic waves in a piezoelectric material are

$$\mathrm{T} = \mathrm{C_e}.\mathrm{S} - \mathrm{et}.\mathrm{E} \qquad (1)$$

$$d = e.S + \mathcal{E}.E \qquad (2)$$

where T is the stress, C_e is the elasticity matrix, S is the strain, e is the piezoelectric coupling constant, E is the electric field intensity, d is the electrical displacement and Ɛ is the permeability.

1.5 Surface Acoustic Wave (SAW) devices

A surface acoustic wave (SAW) is an acoustic wave which travels along the surface of a material which exhibits elasticity, and its amplitude diminishes exponentially with depth into the substrate. These were first explained by Lord Rayleigh in 1885 [7]. He explained the surface acoustic mode of propagation and also predicted its properties. Surface acoustic wave is a general term given to any mechanical wave whose all or most the energy is concentrated at the surface of solid. Piezoelectric effect is mostly used to produce surface acoustic waves.

SAW based gas sensors are a class of MEMS which depend upon the modulation of SAW to sense a physical phenomenon. The input electrical signal is transduced by the sensor into a mechanical wave which, in contrast to electrical signal, could be easily affected by physical phenomena. The SAW device then converts the mechanical wave back into an electrical signal. Parameters like frequency change, change in amplitude, phase change, change in time delay between input and output electrical signals could be utilized to assess the presence of given phenomena. The frequency range for SAW devices is between 10 MHz and 2 GHz. SAW devices are of many kinds including filters, oscillators and sensors [8]. In today’s time, the most commonly used SAW devices are in electronics and telecommunications.

The fabrication of SAW devices primarily needs the deposition or etching of interdigitated transducers (IDTs) on a piezoelectric material. The fabrication of IDTs is compatible with CMOS process technology, so its large scale production is possible. But most of the piezoelectric materials are not compatible with CMOS technology, therefore MEMS-CMOS technology is used for the integration of SAW devices and its processing unit.

Primarily there are two types of structures of SAW devices. The first one is a two port device and is called delay line while the other is a one port device and is called a resonator [9].

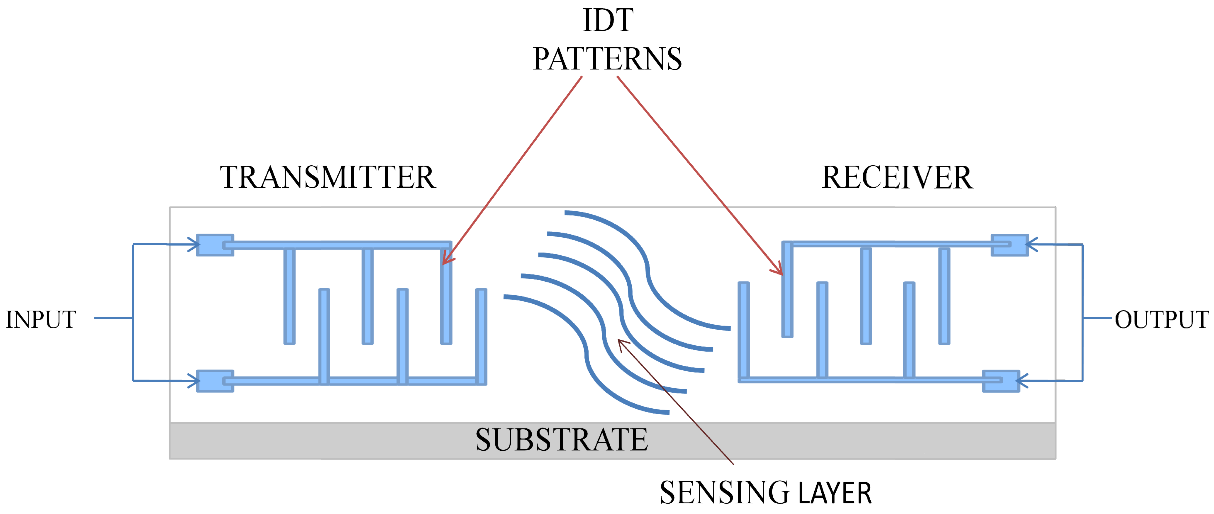


Fig 1.3 Basic structure of two port SAW based gas sensor

The SAW based gas sensor basically consists of a pair of IDTs which are etched on a piezoelectric substrate and are separated by a path called delay path. The acoustic wave travels on the surface on this path and this is where sensing is done. The SAW based gas sensor behaves differently with different types of films and materials used in sensing area. These different films or materials make it work like a different sensor. Furthermore, specially designed IDTs enable the SAW devices to be used as accelerometers and gyroscopes.

The input electrical signal when applied to the IDTs produces an alternating polarity among the fingers of IDT. Between two consecutive sets of fingers of IDT, the polarity will be alternate (like + - +). Therefore the direction of electric field will switch between the adjacent fingers. Due to this alternate regions of strain are created among the fingers of electrode, thus a mechanical wave which is called surface acoustic wave is produced. The distance between the fingers of electrode is known as pitch and it is equal to the wavelength (λ_o) of the mechanical wave. When a signal is applied to the IDT whose period is equal to that of IDT, vibrations occur underneath the IDTs and an acoustic wave is created which travels in direction normal to the direction of IDTs. This acoustic wave travels away from IDTs in both directions with velocity v_o. It penetrates only about half the wavelength into the bulk, rest is concentrated on the surface region. This leads to a high energy density at the surface and therefore the name surface acoustic wave. The operating frequency f_o of the SAW device is related to the wave velocity v_0 and wavelength λ_o as follows [2] :

$$f_0 = \frac{v_o}{\lambda_o} \qquad (3)$$

The velocity by which the wave travels in the piezoelectric material is lower than electromagnetic waves (EM) by a factor of 10^{-5}, hence the SAW wavelength which is transmitted in the substrate is 10^{-5} times smaller than EM waves, therefore making the sensor a compact device. Since the energy in SAW based gas sensor is confined primarily on the surface region, any small changes in the surface conditions will make the input signal different from output signal and thus highly sensitive gas sensors are made using this. Several factors affect the conditions including temperature, pressure, humidity, mass loading etc.

1.6 SAW based gas sensor

The main thought behind the SAW based gas sensor is that a thin gas sensing layer is deposited on the piezoelectric substrate between the two IDTs. The deposition can be done using various techniques like RF sputtering, DC sputtering etc. SAW based gas sensor is effectively similar to other SAW based gas sensors, just that the sensing layer is deposited for detecting specific gas or gases in an area. The alterations in the SAW phase velocity and attenuation are monitored by SAW based gas sensors. These changes occur when gas interacts with the sensing layer and are measured by calculating the frequency and the insertion loss of the SAW based gas sensor. SAW based gas sensor response is dependent on a number of effects which include mass loading, acoustoelectric coupling, viscoelastic loading etc [10]. Typically, SAW based gas sensors utilize one or more of these effects to produce a response.

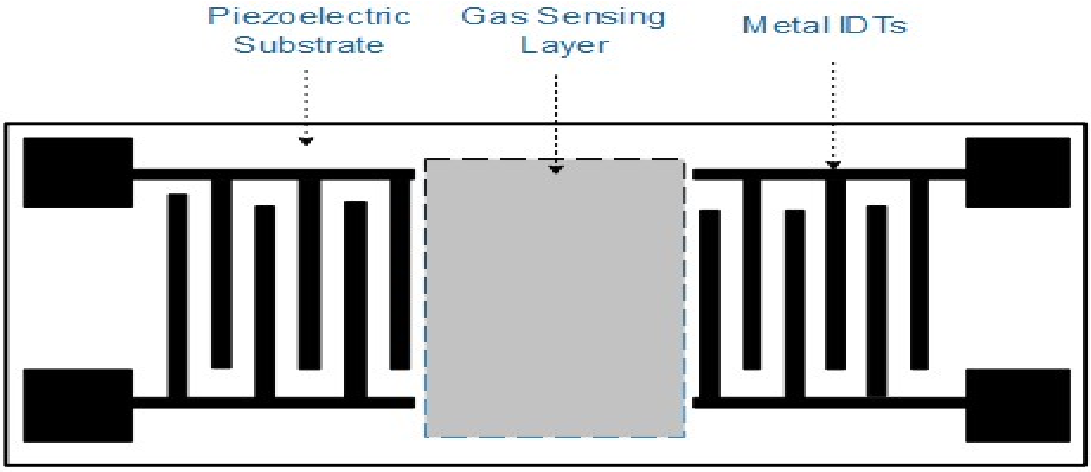


Fig 1.4 Top view of the SAW based gas sensor

1.6.1 Working principle of SAW based gas sensor

SAW based gas sensors use the piezoelectric effect in its operation. SAW based gas sensors use IDTs to convert electrical signal to a mechanical acoustic wave and vice versa. In case of conversion of electric signal to a mechanical wave inverse piezoelectric effect is used while in case of conversion of mechanical wave into an electrical signal piezoelectric effect is utilized.

This wave propagates from input IDT to the output IDT. When this propagating SAW is perturbed, the wave velocity changes, and this could be measured by measuring the frequency shift or the phase shift. The measurement of this perturbance is the main idea behind SAW based gas sensor.

1.6.2 Sensing mechanisms

To develop a SAW based gas sensor, it is really important that sensing mechanism of interaction between sensing layer and analyte gas is understood. The most used sensing mechanism is gravimetric, in which a change of velocity of wave occurs due to adsorption of mass on the structure. Other commonly used mechanisms are in which the change in density, viscosity, permittivity or conductivity of the sensing layer is observed.

In mass based gas sensing, the analyte gas when adsorbs on the sensing layer causes mass perturbations. Surface acoustic waves are strongly guided by the substrate and their sensitivity towards mass perturbations is very high. Mass sensitivity depends upon the thickness of the sensing layer. The mass sensitivity of layered structures is better than non layered counterparts.

During propagation of SAW, the mechanical wave is accompanied by a layer of bound charge. This is called acoustoelectric effect and this is linked to electrmechanical coupling coefficient (K^2) of the material. In conductivity based gas sensing, the electrical boundary condition at the surface is perturbed when an analyte gas interacts with the sensing layer. As a general rule, larger the K^2 of the material, the greater the change in wave velocity due to conductivity changes at the surface.

1.7 Nanotechnology

Nanotechnology is used for functional structures which has at least one characteristic dimension in nanometers. At this scale the properties of materials are unique and could be greatly altered. The properties are usually different from those of atomic scale or of bulk materials. Nanotechnology has a significant impact on sensor technology. It has unique advantages and improves sensitivity, which is the major reason for its use in SAW based gas sensors [11].

Nanostructure material has greater surface area to volume ratio as compared to thin film devices. By improving the morphological and structural properties of nanomaterials, we could get devices with better sensitivity and selectivity. In addition nanostructures also improve the response time of the device. Nanostructured metal oxides as nanorods, nanoparticles, nanobelts and nanorods are the most used nanomaterials.

1.8 Need of SAW based gas sensor

In today's busy industry, health and safety are a crucial part. Accidents should be avoided as these not only cost money and time but also human life. For detecting unwanted, dangerous gases at workplaces, gas sensors are used. These sensors must have some basic properties so as to serve the purpose in best way [12].

Firstly the gas sensor must be uncomplicated and cheap. This means the manufacturing of the device must be simple and also the cost must be low.

Secondly, the sensor must be sturdy. Since sensors could be used in remote areas, it should withstand the wear and tear with time.

Thirdly, the size of the sensor should be small. In today's world, smaller is better. Everyone wants a compact device which should be portable.

Finally, the sensor has to be accurate. Since the gas sensor has to be used as a safety precaution against harmful gases, it must be accurate and should alarm the concerned party before there is any danger to human life.

All the above requirements are fulfilled by SAW based gas sensors. For example catalytic sensors are very stable and can work in a range of temperature and humidity conditions but they are very prone to poisoning which will permanently damage them. Similarly metal oxide sensors are quite useful in places where the harmful gases or hazards are unknown. But to their downside, they are not very accurate and their range is limited. SAW based gas sensors are an excellent proposition for gas sensing. These are small in size, cheap, very sturdy, highly sensitive especially with nanomaterials and highly accurate. These can also work in passive mode i.e these do not need any batteries.

1.9 Structure of SAW based gas sensor

Basic layers of SAW based gas sensor are given below:

1. Substrate

2. Intermediate layer
3. Interdigitated Transducers (IDTs)
4. Sensing layer

Substrate

Substrate, also known as wafer, is the lowermost or the bottom layer of the device and it provides base for the sensor. Piezoelectric materials are used as substrate like quartz, $LiNbO_3$, $LiTaO_3$ etc.

Interdigitated transducers

The comb-like structure which is patterned on the substrate using certain metals is known as Interdigitated Transducer (IDT). Normally there are two sets of IDTs in a SAW based gas sensor; one is at the input and the other at the output. These convert electrical signal into acoustic wave and vice versa. By varying the width, length and thickness of IDTs, sensor performance can be affected.

Intermediate layer

The intermediate layer is preset between the substrate and the sensing layer. Most commonly used materials for this are dielectric materials. It provides the confinement or waveguide at the substrate surface for the acoustic wave. It is also responsible for other properties like sensitivity of the sensor too.

Sensing layer

Sensing layer is very important part of the gas sensor. It is deposited between the IDTs and this is where the sensing mechanism takes place. Different sensing layers are used for sensing different gases.

As presented in the table 1.1, a few of the SAW based sensors are mentioned with different structures and sensing layers to sense different gases [13-16]. Some of the presented sensors have conventional design while some has the layered structure.

Table 1.1: SAW base gas sensor device comparison

Device type	Sensing layer	Structure	Test gas	Device Frequency (MHz)
SAW	WO_3:Ru	24° rotated Y-cut quartz	3ppm of NO	261
SAW	Doped WO_3	YZ $LiNbO_3$	30ppm of H_2S	60
SAW	WO_3:Au	YZ $LiNbO_3$	100ppm of H_2S	38.15
SAW	Langmuir blodgett films	-	1.4ppm of NO_2	600
SAW	lead phthalocyanine	YZ $LiNbO_3$	10ppm of NO_2	110
SAW	catalysed lead phthalocyanine	YZ $LiNbO_3$	10ppm of NO_2	110
SAW	tetra-4-tert butyl silicon phthalocyanine dichloride	ST quartz	100ppm of NO_2	98.6
SAW	lead phthalocyanine	YZ $LiNbO_3$	3.1ppm of NO_2	43
SAW	WO_3	27° quartz	10ppm of H_2S	260
SAW	WO_3	YZ $LiNbO_3$	27ppm of H_2S	60
SAW	Pt/WO_3	Langasite	1000ppm of H_2	167.14
Layered SAW	ZnO	ZnO/90° rotated ST quartz	50ppm of O_2	90
Layered SAW	ZnO	ZnO/90° rotated ST quartz	100ppm of C_3H_8	90
Layered SAW	Palladium	copper phthalocyanine/YZ $LiNbO_3$	2% of H_2	-
Layered SAW	Palladium	phthalocyanine/ YZ $LiNbO_3$	2% of H_2	-
Layered SAW	copper phthalocyanine	SiO_2/90° rotated ST quartz	1ppm of NO_2	100

1.10 Overview of hazardous gases

Hazardous gases are those gases that are considered dangerous to human health when present in excess proportion. They are broadly divided in to two categories: Toxic gases: Toxic gases are those which are potentially harmful to humans when are inhaled. This includes gases like ammonia, chlorine, sulphur etc. Flammable gases: Flammable gases are those which have the potential to burn in certain concentrations. They will burn when oxygen is present around; which usually is; as without oxygen there is a problem for workers around. In addition to the various hazardous gases, there are also sensors which are used to detect the low levels of oxygen which is an essential gas. A summary of various properties of the hazardous gases are shown in Table 1. TLV is the threshold limit of a particular gas that is allowed for repeated exposure without causing any health issue [17]. Nitrogen dioxide (NO_2) which has the TLV of about 3 ppm is very harmful. Hydrogen sulfide (H_2S) is one of the most dangerous gases, as it can disrupt the oxygen supply. It can be detected easily at lower concentrations from its rotten egg like smell but at higher concentrations, it affects the senses badly, and one is not able to sense it. Carbon monoxide (CO) is a colourless and odourless gas and is undetectable without a sensor. Ammonia (NH_3) is a colourless gas with pungent odour. It is harmful to human health when its concentration reaches more than 25 ppm. Health effects due to excessive exposure of sulphur dioxide (SO_2) include respiratory problems. Persons with asthma are sensitive to it. Methane (CH_4) can explode in air when present below 5%. Nitrous oxide (N_2O) creates global warming to a large extent which causes disruption in ozone layer. Carbon dioxide (CO_2) is a colourless and odourless gas. It is emitted by human activities. Environmental monitoring of these gases is must to ensure a good environmental health. One-third of carbon dioxide is emitted during transportation[18]. The use of fossil based fuels emits greenhouse gas and also degrades air quality. According to the pollution index rating 2016, out of top ten polluted cities in the world; three are Indian cities, which is definitely an issue of major concern. Demand of energy is increasing and the condition of fossil fuel supplies is at gloom. Hydrogen (H_2) energy is renewable and pollution-free. Water vapour and heat are the by-products of hydrogen energy, not any other air pollutant. Because of these advantages, hydrogen fuelled products becoming popular. Safety is the most important issue that needs to be taken care while its development. The explosive range of hydrogen is from 4% to 74%. Therefore, hydrogen sensors should carefully monitor the hydrogen leak for safe use of hydrogen energy.

Table 1.2 Properties of various hazardous gases

Gas	Physical property	Source of emission	Environmental/health impacts	TLV
No2	Reddish-brown in colour, pungent odour	Mostly from automobile and industrial sector	Respiratory problems, corrode metals	3 ppm
NO	Non-flammable	Produced during combustion in air	Irritation in eyes	25 ppm
N2O	Colourless with a sweet odour	from nitrogen fertilizers, and from oceans	Causes greenhouse effect	50 ppm
H2S	Colourless, toxic and flammable in nature rotten egg smell	through volcanic gases and hot springs	Effects breathing	10 ppm
CO	Colourless, odourless, non-irritating gas .	Through incomplete carbon products like wood, coal.	Prevents absorption of oxygen in blood thus damaging vital organs	50 ppm
NH3	Colourless, pungent odour	During the decomposition of animal manures	Irritation in eyes	25 ppm
CH4	Odourless and Combustible gas	By an-aerobic digestion of organic materials	Explosive	1000 ppm
SO2	Lighter than air, Invisible gas with nasty smell	Produced from industrial emission	Irritation in nose, throat, and causes Shortness of breath, and heaviness in chest.	5 ppm
CO2	Colourless and odourless gas	Vehicle emissions	Creates suffocation and oxygen deficiency	5000 ppm
H2	Light, Non-toxic, odourless, highly flammable, easily reacts	Cylinders,lpgtanks,pipelines	High concentration causes oxygen deficient environment which leads to breathing shortness, exploxive mixtures easily formed	Flammability limit 4%-75%

1.11 Thesis organization

Chapter 1 gives introduction about sensors and their use in daily life. It briefly explains the gas sensors and the use of MEMS technology in these. Then the SAW devices as well as SAW based gas sensor are explained. The structure and working of SAW based gas sensor is explained and also the use of nanotechnology in these gas sensors. In the end an overview of some hazardous gases is provided.

Chapter 2 provides the information regarding the works performed till date. The literature survey clearly shows the advancements in the field of SAW based gas sensors with recent updations for the enhanced performance of sensor. The various outcomes from the literature survey had been studied and the objectives that can be fulfilled in the stipulated time have been studied using simulation tools as well as upto an extent with fabrication.

Chapter 3 deals with the introduction of the simulation tool used in the study. The studies performed using the simulation tool are elaborated with each step included. Various steps regarding the selection of physics, geometry, mesh settings and much more are clearly mentioned and explained with the steps included with them.

Chapter 4 presents the designing of the SAW based sensor using the simulation tool. The different models including various architectures for a particular ZnO based hydrogen gas sensor has been studied. The chapter shows the modelling and simulation of the designing part of the sensor.

Chapter 5 concludes with the various simulation results for the sensor. The simulation results present the various important parameters which can be helpful for optimising some parameters such that the fabricated sensor shall have an improved performance.

Chapter 6 includes the various steps involved in the fabrication of the SAW based sensor that are performed in the lab. The steps presents the fabrication of basic architecture for a sensor which shows the procedure to be followed for a SAW based gas sensor.

Chapter 7 concludes the present study and suggests the parameters that can be varied in accordance for the improvement of a gas sensor with the works that can be performed in future.

CHAPTER 2

LITERATURE SURVEY

This chapter focuses on the study of the work done by various other researchers in the field of SAW based gas sensor. Various developments over the period of time have been studied. The objectives of the present study are finalized according to gaps present in the study at the end of the chapter.

- Slobdnik A.J. in 1976 received the material parameters which are required for the optimal design of Surface Acoustic Wave (SAW) devices. The parameters include wave velocity, coupling coefficient, temperature coefficients and propagation loss. Sufficient theoretical information for the full understanding and for deriving properties and parameters cited above is given. A succinct tabular summary of important properties of SAW materials is provided [19].

- Joshua J. Caron et al. in 1995 studied the different orientations of substrate materials of SAW based gas sensors. Earlier works have focused on the sensing layer and gas-sensing layer interaction. For identifying temperature stable substrate, a systematic study of different orientations of quartz was made. Experimental data on different 4-cuts in quartz is in accordance with the theory. An H_2S sensor that has an operating temperature of $200^{\circ}C$ has been fabricated using 27° rotated 4-cut quartz which shows higher stability to SAW based gas sensors using YZ $LiNbO_3$ substrates [20].

- Y.J. Lee et al. in 1998 developed a new type of SO_2 SAW based gas sensor by using inorganic thin film. At that time, SO_2 gas sensors were quite costly and somewhat complex. Cadmium Sulphide (CdS) thin films were used as new detection material for SO_2. Substrate material used was $LiTaO_3$. Sensor properties like sensitivity, response time and repeatability were tested. The sensor showed encouraging performance and worked at 54 MHz center frequency and measured concentration of less than 200 parts per billion of SO_2 in air at 160°C [21].

- Vladmir I. Anisimkin et al. in 1998 investigated new properties of SAW based gas sensors. They found that on exposing the SAW based gas sensor, the response can be increased, decreased, fastened, and slowed for a particular selected sensitive layer by simply altering the substrate material and orientation. Experimental results were produced for quartz substrate coated with polycrystalline palladium when exposed to different gases like H_2, CO, N_2O at different concentrations of humidity in air [22].

- Kourosh Kalantar- Zadeh et al. in 2002 fabricated a new layered SAW based gas sensor. They used 90^o rotated ST-cut quartz crystal at substrate and ZnO layer. The sensor was used for gas as well as liquid sensing. Sensor response was tested for varied inputs of oxygen in nitrogen gas. The sensor could sense gas concentrations as low as 0.2 ppm of O_2 gas in nitrogen gas [23].

- S. Ahmadi et al. in 2004 designed a SAW based gas sensor with $LiNbO_3$ base and ZnO thin film base which was highly selective and sensitive. Different structures like single layer (ZnO) and multi-layer (ZnO/ SiO_2/ Si) were designed and simulated for different thickness of ZnO film. Simulation and experimental results of the SAW based gas sensors were provided and compared [24].

- S.J Ippolito et al. in 2006 proposed a design for layered SAW based gas sensor with 36^o YX $LiTaO_3$ substrate with 1.2 μm ZnO layer as intermediate layer and 150 nm Tungsten trioxide (WO_3) as sensing layer for ethanol. Sensor performance produced a response as function of operating temperature and relative humidity (RH). Observed frequency shifts were 119, 90 and 86 KHz for 0, 25 and 50 % RH and this was done for 500 ppm of ethanol in air. Response decreased with increase in RH and decrease in operating temperature [25].

- A.Z. Sadek et al. in 2006 has fabricated a novel sensor. The sensor was based on a polyaniline/ In_2O_3 nanofibre composite and used ZnO as intermediate layer and 64^o YX $LiNbO_3$ as substrate. The nanocomposite had been deposited on a layered structure of ZnO/ $LiNbO_3$. The sensor was exposed to gases including H_2, CO_2 and NO_2. The sensor showed good repeatability and had fast response and recovery times at 25°C [26].

- N. Wlodarski et al. in 2007 presented and developed a layered SAW based gas sensor for hydrogen gas which was ZnO nanorod based. The ZnO nanorods had been deposited on a layered structure of ZnO/ 64^o YX $LiNbO_3$. Gold was used for electrode and the diameter was kept around 100 nm for ZnO nanorods. Operating temperature was kept between 200°C and 300°C. The sensor produced highest frequency shift of 274 KHz at 265°C for 0.15% H_2 [27].

- Guigen Zhang in 2009 reviewed the basic principles of SAW devices and SAW-based Love mode sensors and illustrated that there was a need for improvement in active area of SAW based gas sensor. COMSOL software was used to provide an example of SAW based gas sensor incorporating nanopillars. The simulated results show that nanopillars increase active surface area and sensitivity of SAW based gas sensors gets increased [28].

- Peng Zheng et al. in 2009 simulated a layered SAW based gas sensor using 'COMSOL' software. The layered structures used in the set up were ZnO/ Si_3N_4/ $LiNbO_3$ and ZnO/ SiO_2/ $LiNbO_3$. The motive was to analyze the effect of change in thickness and composition of the spacer layer and the sensing layer on the sensitivity of the SAW based gas sensor. The results show that the sensitivity was maximum when the spacer layer was thin and the sensing layer gets thicker. The two layered structured were also compared at different thickness [29].

- N.A. Ramli et al. in 2011 studied the key design parameters on which the performance of SAW based gas sensor is dependent like spacing between IDT and reflector, optimum spacing between the electrodes (IDTs) and the number of reflectors to get highest mechanical displacement. The optimization of these parameters provides precise resonant frequency (fr), low insertion loss and high Quality factor (Q) which is the key for a SAW based gas sensor. FEM simulations were performed to optimize the SAW based gas sensor design [30].

- Gouthami N et al. in 2011 proposed a 3D model of SAW based gas sensor for sensing hydrogen gas. The model introduced nanowires in sensing area to improve conductivity. A layered structure based on ZnO/ $LiNbO_3$ was used. The thickness of intermediate layer was varied to optimize the design. The introduction of nanowires improved the performance and sensitivity of the sensor and optimum width of ZnO layer was found out [31].

- N.J.L Muniraj et al. in 2011 simulated a 3D SAW based gas sensor for detection of dichloromethane (DCM). Lithium Niobate ($LiNbO_3$) is used as the substrate and

PolyIsobutylene (PIB) as the sensing layer. PIB will selectively adsorb DCM from air and this leads to increase in mass of PIB film. This causes a shift in resonance frequency and lowers it slightly. Hence, DCM can be detected using this sensor [32].

- Chunbae Lim et al. in 2011 developed a SAW based multi-gas sensor which simultaneously detected CO_2 and NO_2. 41° YX $LiNbO_3$ was used as a substrate. The sensor consisted of an IDT, 10 reflectors, Teflon AF 2400 as CO_2 sensitive film and Indium Tin Oxide (ITO) for NO_2 sensitive film. The sensor showed good repeatability and linearity. The sensitivities obtained for CO_2 and NO_2 were 2.12°/ ppm and 51.5°/ ppm respectively [33].

- Xianping Chen et al. in 2013 studied and reviewed the recent developments of nanotechnology in SAW based gas sensors. Nanowires as sensing elements are powerful as these have many improved characteristics like high surface to volume ratio, ultrasensitivity, high selectivity, quick response and less power consumption. Top-down and bottom-up approaches for synthesizing nanowires were compared. An emerging fabrication method and a nanowire pH gas sensor which is self powered was discussed [34].

- H.G. Du Plessis et al. in 2013 presented a 2D SAW based gas sensor in which ZnO nanopillars were added to the sensing area. 128° YX Lithium Niobate ($LiNbO_3$) was used as substrate. The simulations were done on COMSOL software. Frequency and time dependent studies were carried out on the device. The optimal height for electrodes was determined [35].

- Staline Johnson and Dr. T. Shanmuganantham in 2014 designed and analyzed a SAW based gas sensor to detect volatile organic gases. YZ cut Lithium Niobate ($LiNbO_3$) was used as substrate material, Aluminium (Al) was used as material for electrodes of IDT and PolyIsoButylene (PIB) thin film was used as sensing layer. COMSOL tool was used for carrying out the simulations. Mass loading effect was primarily used for detecting the presence or adsorption of gases on sensing layer. Various organic gases like chloromethane, carbon tetrachloride etc were tested and sensor was exposed to 100 ppm of these gases. Frequency shift in various gases was determined [36].

- S. Trivedi et al. in 2015 designed a 3D love wave based SAW based gas sensor. The device is based on 36° YX Lithium Tantalate substrate on which SiO_2 layer acts as waveguide. Mass sensitivity and Insertion loss were observed. The device gave mass sensitivity of 83.22 m^2/kg. This was consistent with previous results [37].

- K.M. Mohibul Kabir et al. in 2015 compared a SAW based gas sensor with microbalance based sensor. Quartz was used as substrate in both cases and gold layers as electrodes. Mercury (Hg) vapours were used to test the sensitivity and performance of these sensors. Results showed that SAW based gas sensors had faster response time, better selectivity and better sensitivity than microbalance based sensor [38].

- G. Matthews et al. in 2016 studied a novel approach to analyze SAW devices based on series of 2D Finite Element Method (FEM) simulations. Two SAW structures having Lithium Niobate ($LiNbO_3$) as substrate and different number of electrodes in their Inter Digital Transducers (IDTs). Then, the SAW devices were fabricated based on those simulations and the measured responses of frequency were found to be very in accordance with simulated results [39].

- M.D. Nazibul Hasan et al. in 2016 fabricated and simulated a 2D layered SAW-based gas sensor for hydrogen gas sensing. A ZnO nano multilayer structure was suggested to improve the sensitivity of SAW based gas sensor. Different materials are considered for intermediate layer. By varying the aspect ratio of the nanorods, the height or thickness of intermediate layer and distance between electrodes, frequency shift and total displacement could be improved greatly [40].

2.1 Objectives of the study

The objectives for the present work are as follows:

1. To design a SAW based gas sensor having layered structure using COMSOL Multiphysics software.
2. To incorporate nanostructure thin films as sensing elements and to compare the results with layered structure.
3. To optimize the thickness of intermediate layer for better sensitivity.

CHAPTER-3

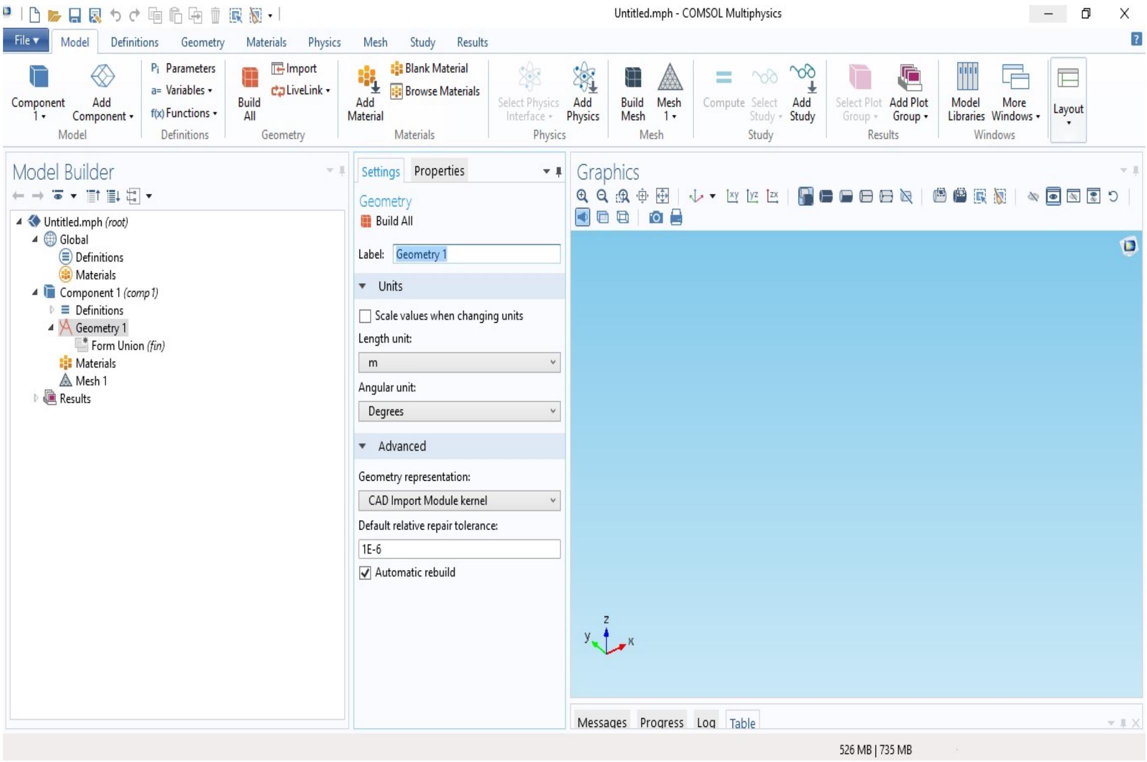
INTRODUCTION TO COMSOL MULTIPHYSICS

This chapter introduces the tool used for the present study. Basic information about the tool is provided in this chapter. Also the various steps required for the study are explained clearly.

3.1 COMSOL MUTIPHYSICS

COMSOL Multiphysics is simulation software and was founded in Sweden and used worldwide for various applications. It includes packages for engineering and medical applications. The purpose of the tool is to create a virtual environment for a particular task to get the similar results as of the real environment. It has various modules like AC/DC module, MEMS, electrical, chemical, plasma, general physics etc. In this software multiple physics are included at the same time to design and simulate any geometry and this is the reason it is called Multiphysics.

It includes various interfaces and properties of different materials. Users can propose their own variables and equations. Shown below in fig 3.1 is the main window of COMSOL.



Label: Geometry 1

Units

☐ Scale values when changing units

Length unit: m

Angular unit: Degrees

Advanced

Geometry representation: CAD Import Module kernel

Default relative repair tolerance: 1E-6

☑ Automatic rebuild

526 MB | 735 MB

Figure 3.1 Interface of COMSOL

3.2 Steps to model

Given below are the basic steps which are required to set up a model.

Step 1

At opening of the COMSOL (5.2), two options are asked by the tool:

1) Model Wizard
2) Blank Model

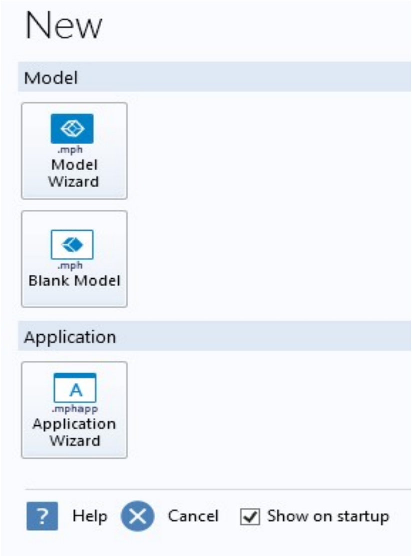


Figure 3.2 Selecting model type

Working in model wizard

The model wizard will ask for dimensions to work as shown in figure.

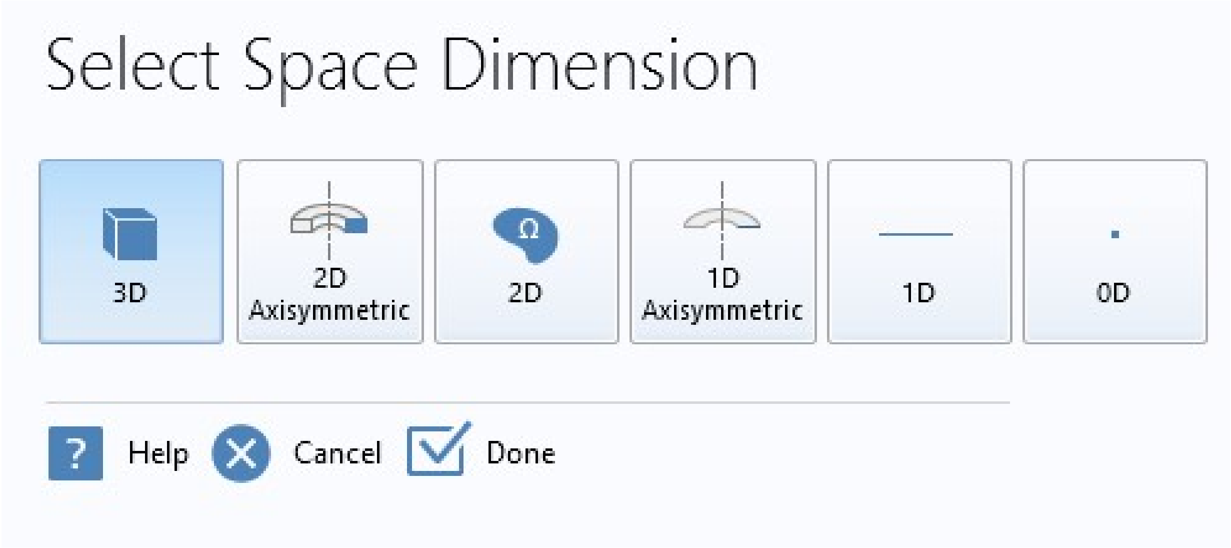


Figure 3.3 Select space dimensions

Step 2

After selecting dimensions, tool will ask to select the type of physics and after selecting that there comes the option of selecting the study.

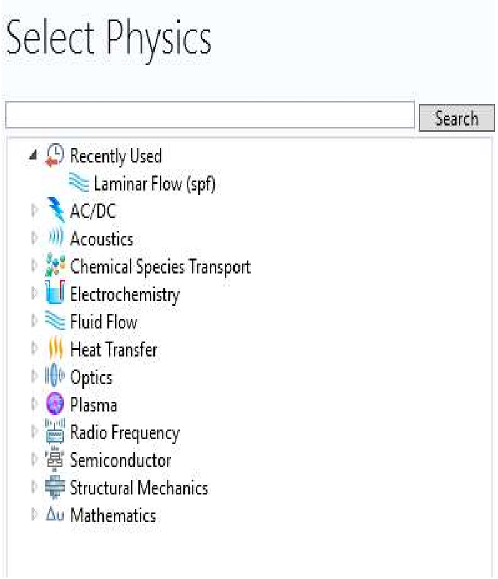


Figure 3.4 Selection of Physics

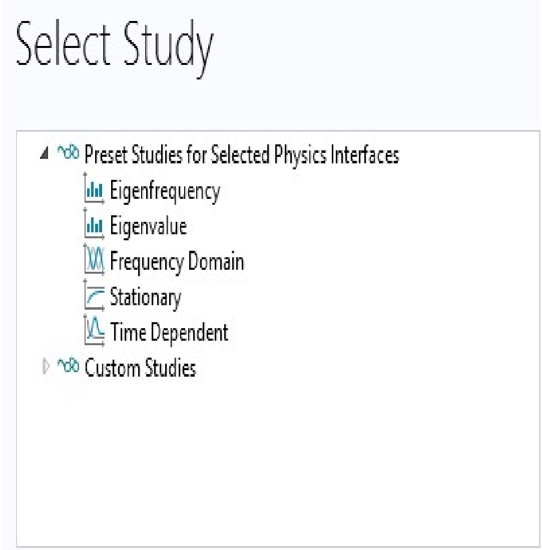
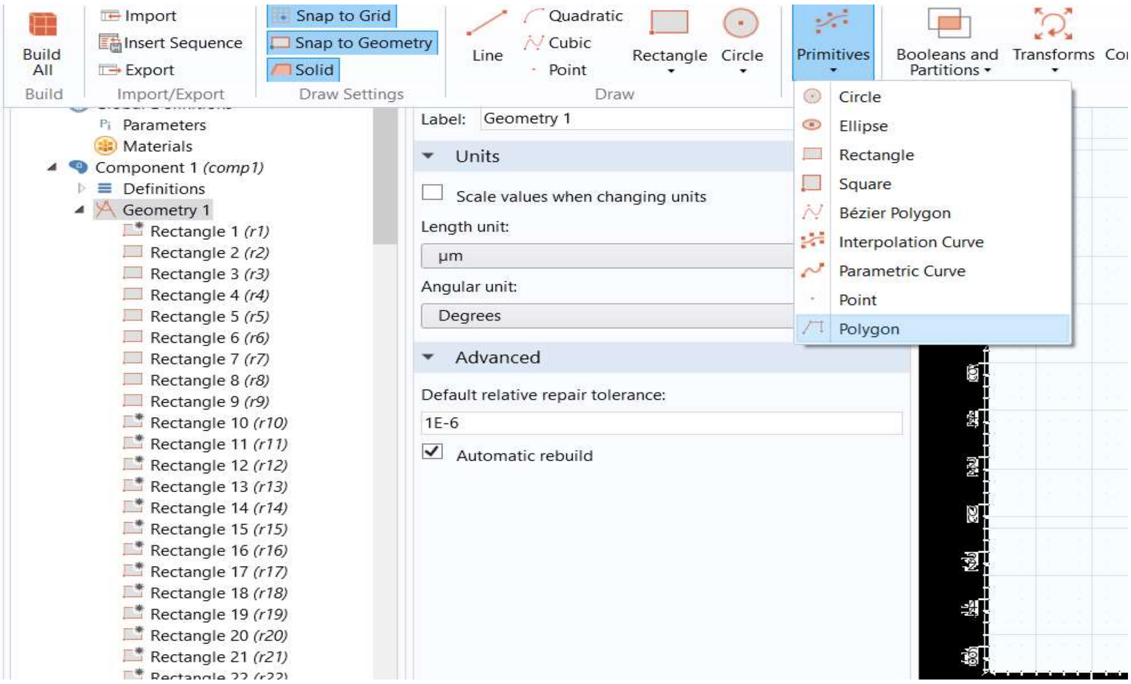


Figure 3.5 Selection of Study

Step 3

Build the required geometry. Different primitive shapes like rectangle, square, circle etc could be used.



Label: Geometry 1

☐ Scale values when changing units

Length unit: µm

Angular unit: Degrees

Default relative repair tolerance: 1E-6

☑ Automatic rebuild

Figure 3.6 Building the geometry

Step 4

Now the materials are added to the different domains of the geometry as per requirement. Many of the materials are inbuilt in the tool's library and could be added directly while other materials which are not available in tool library can also be added by providing their properties.

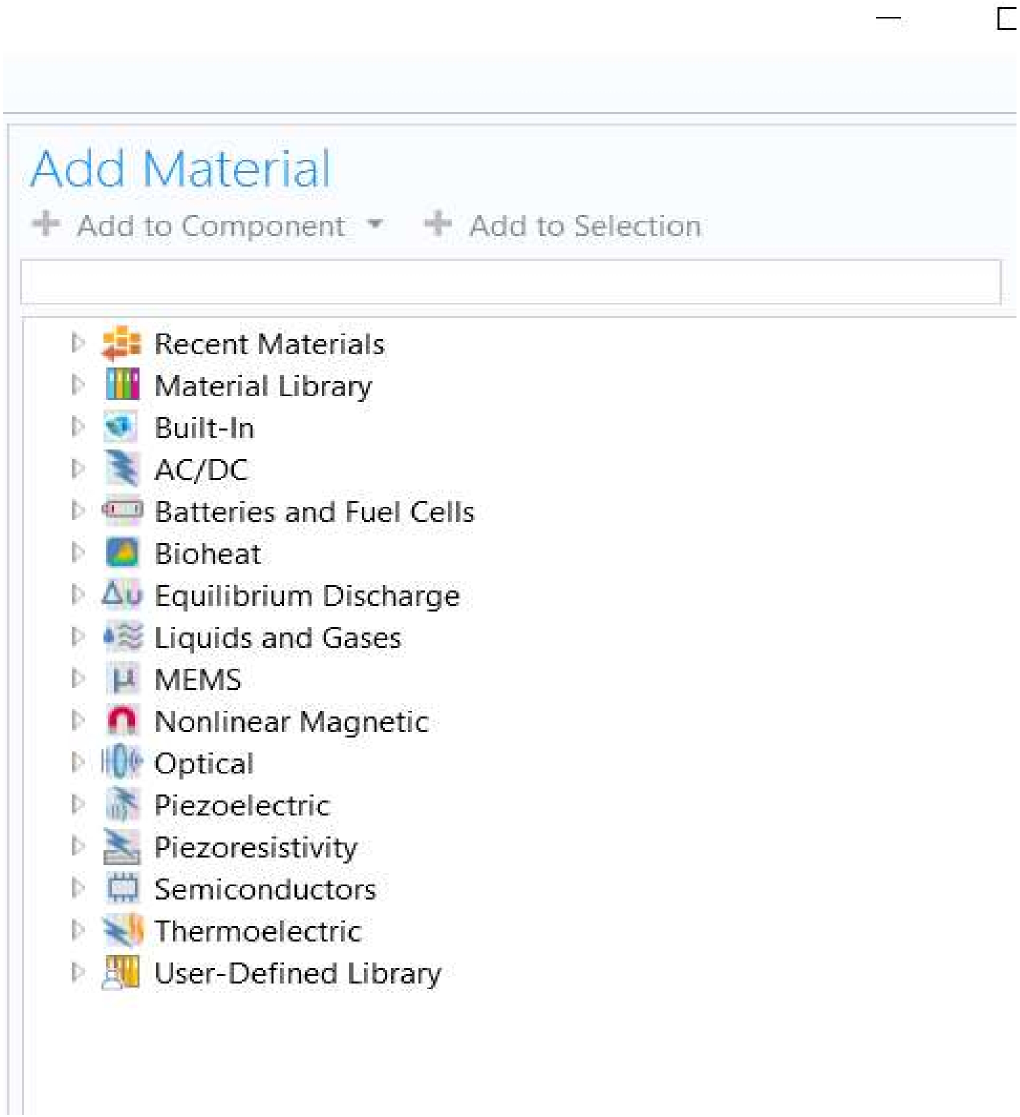
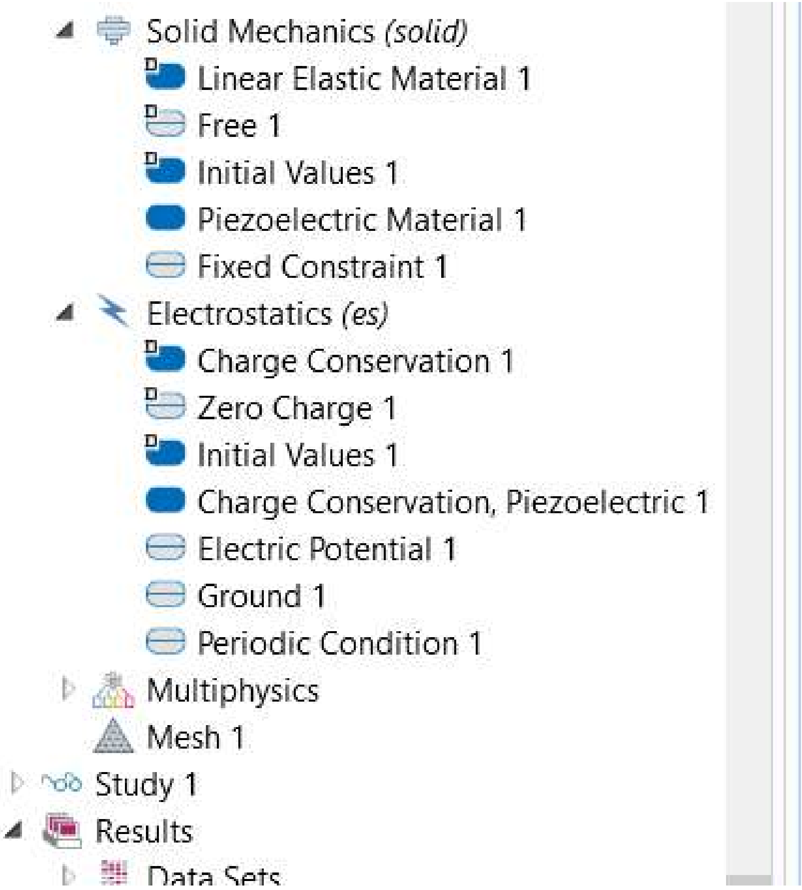


Figure 3.7 Adding materials to different domains

Step 5

Now the physics is to be applied to the model. Various aspects like boundary conditions, terminals, initial values etc are to be specified according to the requirement of the model.

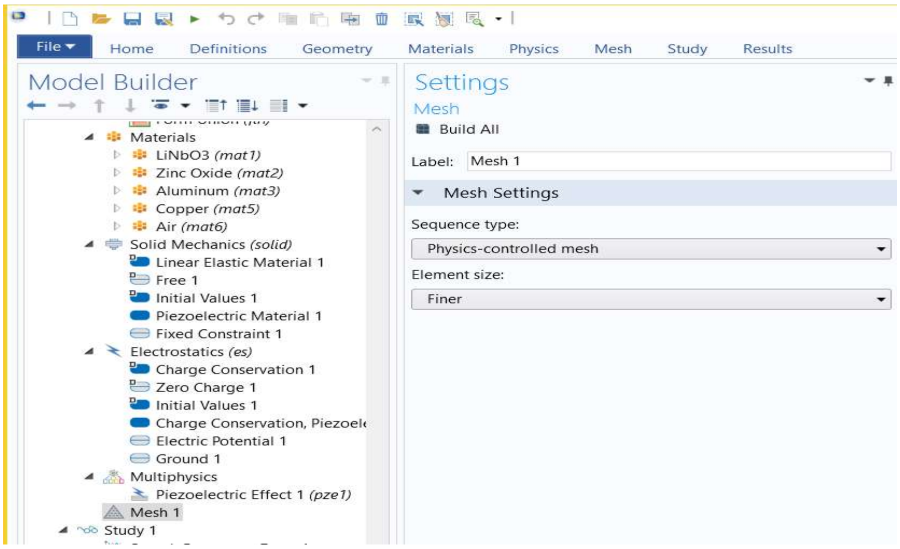


- Solid Mechanics *(solid)*
  - Linear Elastic Material 1
  - Free 1
  - Initial Values 1
  - Piezoelectric Material 1
  - Fixed Constraint 1
- Electrostatics *(es)*
  - Charge Conservation 1
  - Zero Charge 1
  - Initial Values 1
  - Charge Conservation, Piezoelectric 1
  - Electric Potential 1
  - Ground 1
  - Periodic Condition 1
- Multiphysics
- Mesh 1
- Study 1
- Results
  - Data Sets

Figure 3.8 Applying physics

Step 6

Now the geometry or the model is to be meshed. Meshing has to be done carefully as it could take a lot of computational power and time if the meshing part is not done properly.



Label: Mesh 1

Sequence type: Physics-controlled mesh

Element size: Finer

Figure 3.9 Creating the mesh

Step 7

Now the study is to be executed. The study/studies chosen in step 2 are executed in this step by providing the data required for running it.

Step 8

The results are viewed and could be refined by changing parameters etc.

These are fairly simple steps but utmost care should be taken at every step as even a single mistake would lead to lengthy computational times and huge amounts of computational memory wastage and could lead to wrong or inaccurate results.

CHAPTER-4

SENSOR DESIGN

This chapter provides details about the different architectures of SAW based gas sensors used. It also gives details regarding parameters being used to carry out simulations of the present. Different design models of the sensors are also shown in this chapter.

4.1 Introduction

In this project COMSOL Multiphysics 5.2 is used to design and simulate a SAW based gas sensor. Two 2D models of layered SAW based gas sensors are simulated. One is a layered structure which uses thin film as sensing layer as shown in fig 4.1, second is using nanorods as sensing layer as shown in fig 4.2. A 3D model is also simulated find the optimum thickness of intermediate layer so as to optimise the device. All these gas sensors are designed to sense H_2 gas.

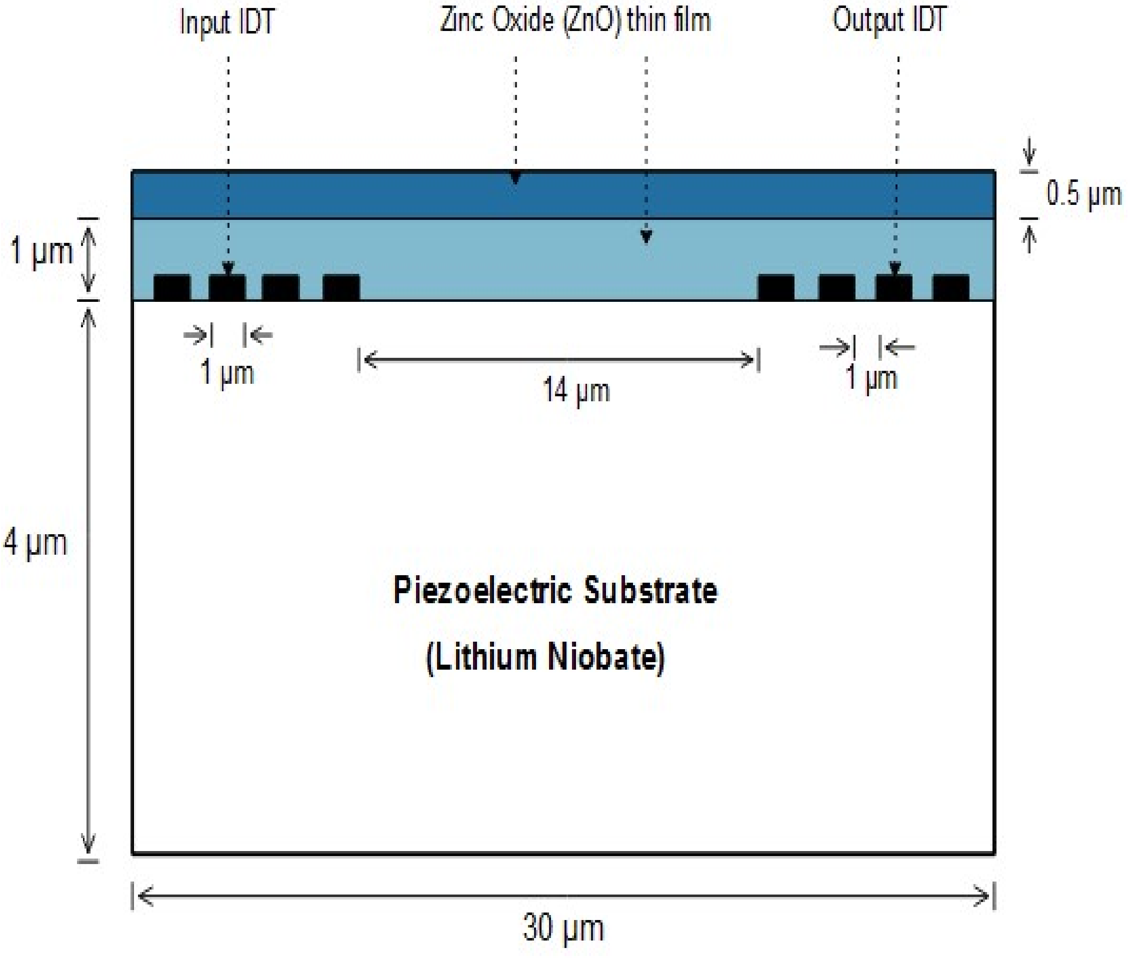


Figure 4.1 Schematic of 2D structure using thin film as sensing layer

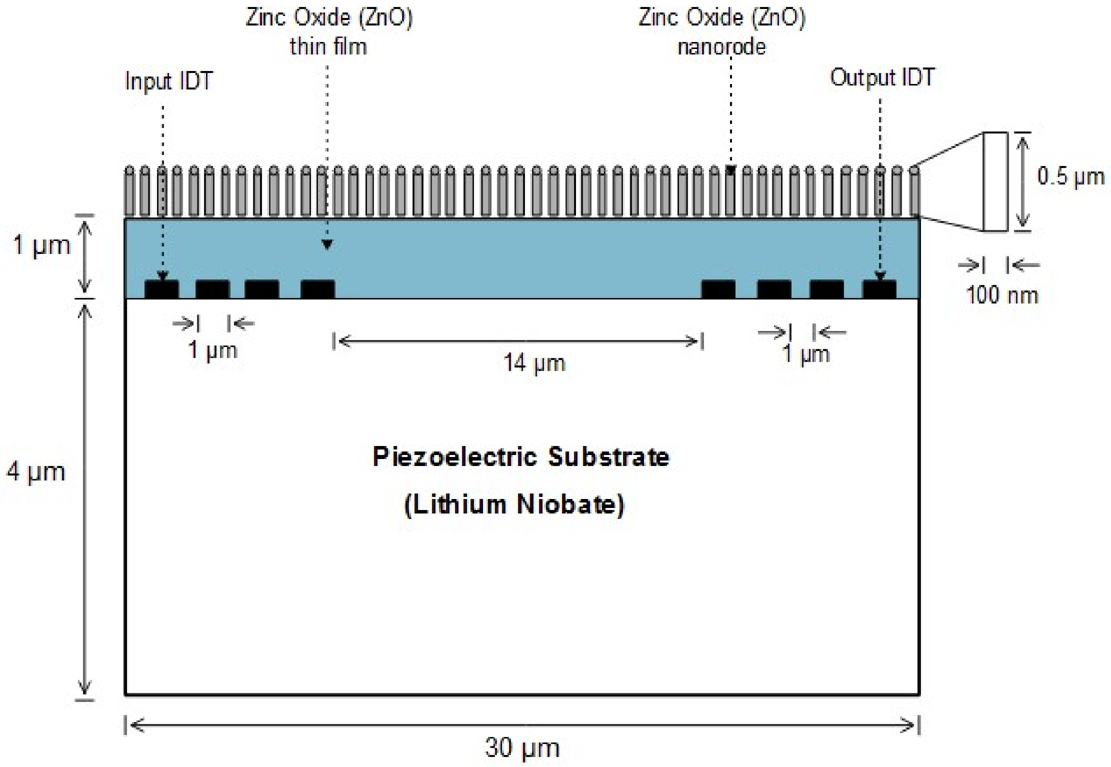


Figure 4.2 Schematic of 2D structure using Nanorods as sensing layer

4.2 Selection of materials for the sensor

Piezoelectric substrate

The substrate material is chosen by considering certain aspects like electromechanical coefficient (K^2), orientation, sensitivity etc. The choice of substrate is a very crucial one. Different materials will give varied performances and sensitivities. So it should be chosen very wisely. For this project, Lithium Niobate ($LiNbO_3$) was selected as the piezoelectric material for the substrate. It has very high K^2 and offers great sensitivity to the perturbations and wave velocity in it is also very high. Specifically YX cut $LiNbO_3$ is used in this.

Intermediate layer

Basically dielectric materials are used as material in intermediate layer like ZnO, PMMC (polymethylmethacrylate), parylene etc. These act as waveguides for the SAW waves. It basically restricts the wave on the surface region so that it shouldn't penetrate deep into the substrate. It should have certain properties like low insertion loss, homogeneity, lower wave velocity than substrate. It should also properly alienate the IDTs from the sensitive layer. Zinc Oxide (ZnO) is chosen in this project as it has very low wave velocity and it improves the sensitivity of the device greatly. The properties influenced by the addition of this layer includes K^2, polarization, phase velocity etc.

Interdigitated Transducer (IDTs)

IDTs are an important component as these convert the electrical signal into mechanical wave. There are many materials like gold (Au), platinum (Pt), aluminium (Al), copper (Cu) etc which could be used as IDT material. Many different materials are tested and the best one is chosen in the end.

Table 4.1 Properties of the IDT materials[41]

	Aluminium (Al)	Copper (Cu)	Gold (Au)
Density (g cm^3)	2.7	8.96	19.3
Young's Modulus (GPa)	70	117	79
Poisson's Ratio	0.35	0.34	0.44
Lame's first parameter (GPa)	58	108	162
Shear Modulus (GPa)	26	48	27
Bulk Modulus (GPa)	76	140	180

Sensing layer

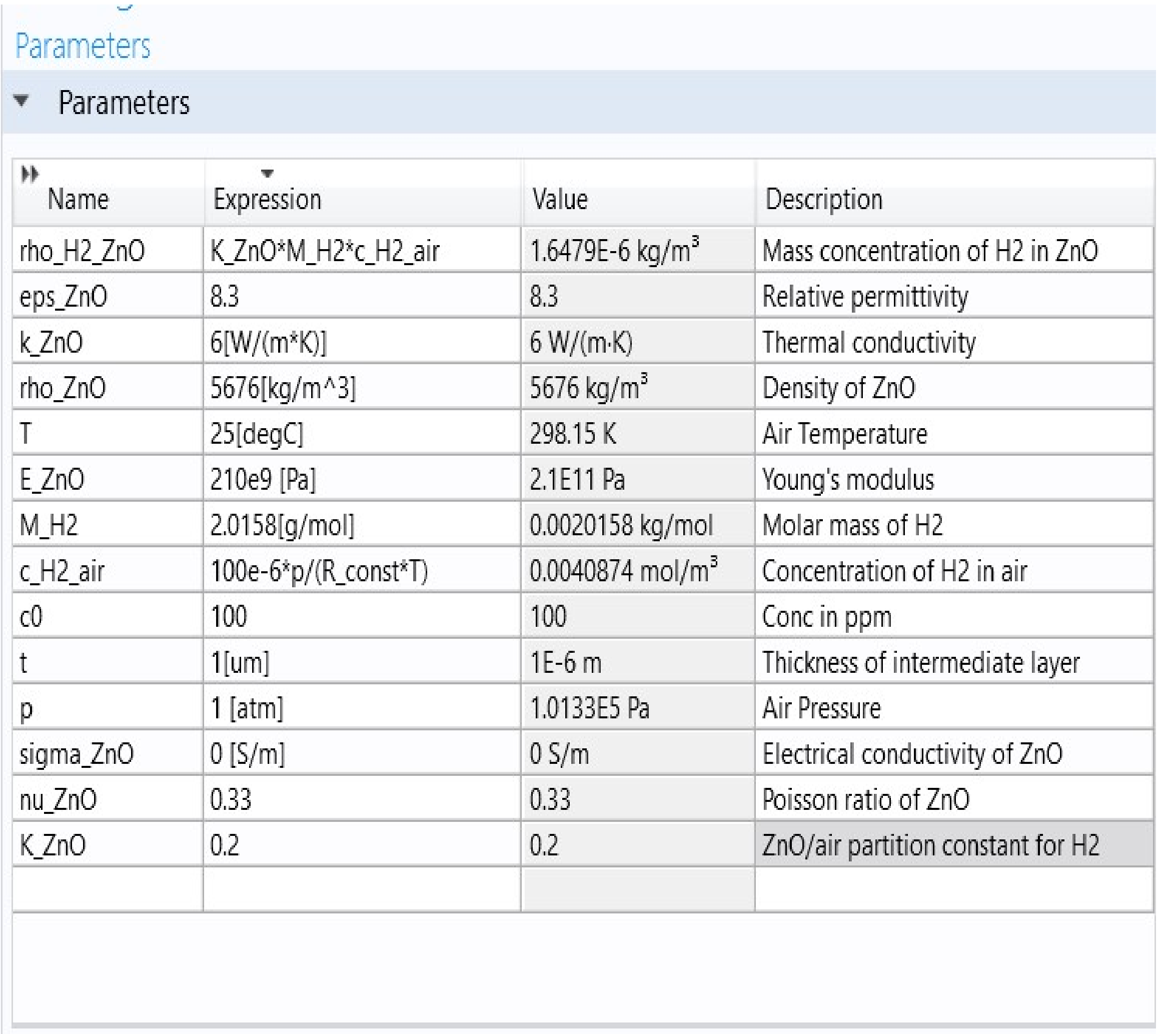
Sensing layer is where the gas sensing takes place, hence it is a very important part of the device. Perturbations due to adsorption of gas occur here. The sensing should be fairly stable and should withstand different chemical and thermal changes. It should also be highly conducting so as to detect even the minute changes to the surface due to adsorption of gas. Here ZnO is chosen as the sensing layer. It has many advantages as compared to other materials which could be chosen. It has very good conductivity and good sensitivity for H_2 gas and it also is an inbuilt material in tool's library.

4.3 Design of the gas sensor

In this project, firstly optimum thickness of the electrodes is determined and also the different materials for IDT are used to compare their results to find the best suited material. Then two gas sensors are designed. One is a layered structure with thin film as the sensing layer and in the other we have used nanorods as the sensing layer. Then a 3D gas sensor is designed using nanorods as sensing layer. The physics used in designing of all theses sensors is Piezoelectric devices multiphysics which combines aspects of solid mechanics with electrostatics. The studies used are eigenfrequency and time dependent.

4.3.1 2D layered structure

For this structure we select 2D in the space dimensions. We use both eigenfrequency and time dependent studies. Before doing any modelling and simulation, we need to define some parameters. These are given below in the figure.



Name	Expression	Value	Description
rho_H2_ZnO	K_ZnO*M_H2*c_H2_air	1.6479E-6 kg/m³	Mass concentration of H2 in ZnO
eps_ZnO	8.3	8.3	Relative permittivity
k_ZnO	6[W/(m*K)]	6 W/(m·K)	Thermal conductivity
rho_ZnO	5676[kg/m^3]	5676 kg/m³	Density of ZnO
T	25[degC]	298.15 K	Air Temperature
E_ZnO	210e9 [Pa]	2.1E11 Pa	Young's modulus
M_H2	2.0158[g/mol]	0.0020158 kg/mol	Molar mass of H2
c_H2_air	100e-6*p/(R_const*T)	0.0040874 mol/m³	Concentration of H2 in air
c0	100	100	Conc in ppm
t	1[um]	1E-6 m	Thickness of intermediate layer
p	1 [atm]	1.0133E5 Pa	Air Pressure
sigma_ZnO	0 [S/m]	0 S/m	Electrical conductivity of ZnO
nu_ZnO	0.33	0.33	Poisson ratio of ZnO
K_ZnO	0.2	0.2	ZnO/air partition constant for H2

Figure 4.3 Parameter constants for designing the sensor

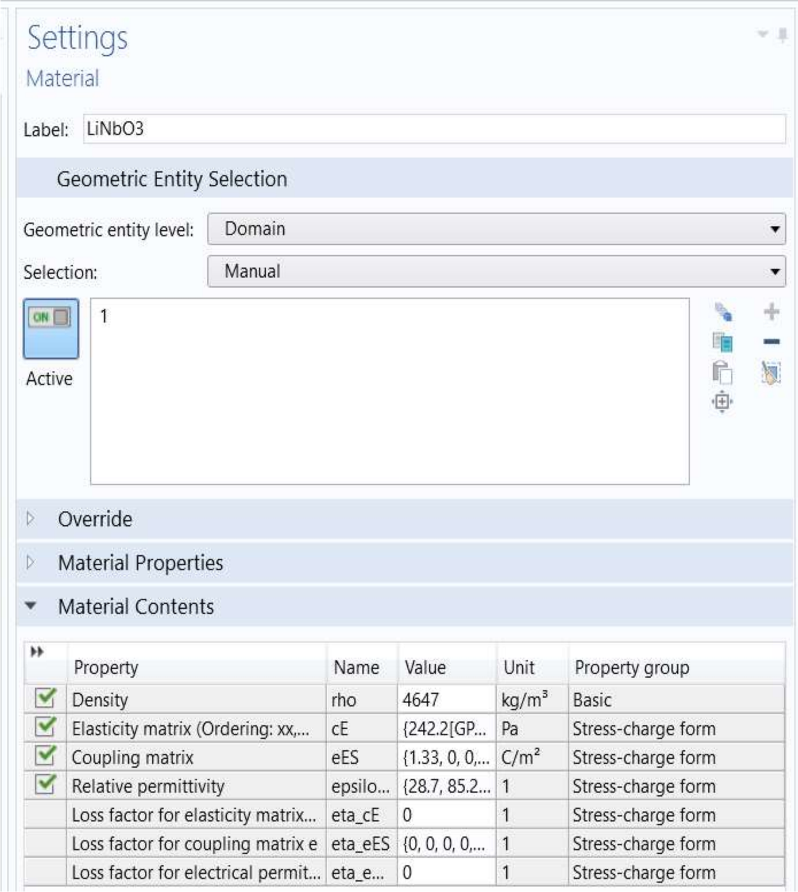
Geometry

The dimensions of the substrate are 30µm*4µm and that of intermediate layer are 30µm*1µm while sensing layer has dimensions of 30µm*0.5µm. The dimensions of IDTs are 1µm*0.2µm and fingers are spaced 1µm apart from each other.

Subdomain setting

Now the materials are to be added to particular domains. We are using $LiNbO_3$ as substrate and it is not an inbuilt material so parameters for it are provided. We also have to provide some parameter constants for other materials too. Different parameters for different domains are shown:

i. YX $LiNbO_3$ substrate



Label: LiNbO3

Geometric entity level: Domain

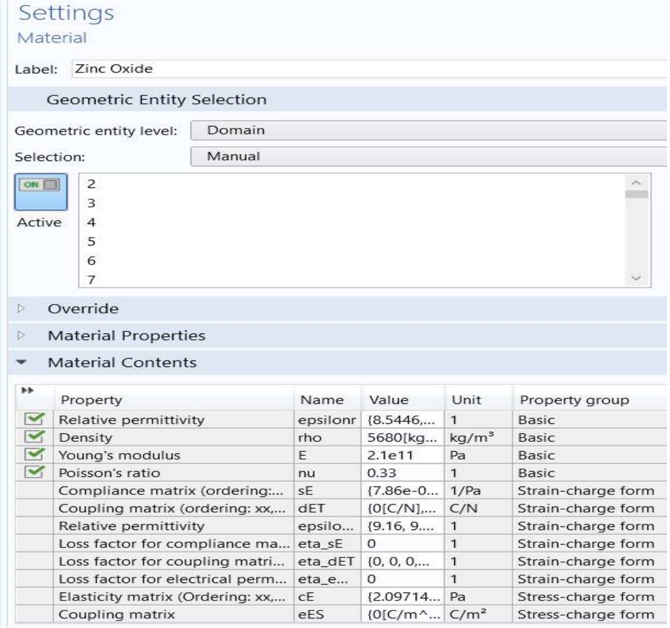
Selection: Manual

1

	Property	Name	Value	Unit	Property group
☑	Density	rho	4647	kg/m³	Basic
☑	Elasticity matrix (Ordering: xx,...	cE	{242.2[GP...	Pa	Stress-charge form
☑	Coupling matrix	eES	{1.33, 0, 0,...	C/m²	Stress-charge form
☑	Relative permittivity	epsilo...	{28.7, 85.2...	1	Stress-charge form
	Loss factor for elasticity matrix...	eta_cE	0	1	Stress-charge form
	Loss factor for coupling matrix e	eta_eES	{0, 0, 0, 0,...	1	Stress-charge form
	Loss factor for electrical permit...	eta_e...	0	1	Stress-charge form

Figure 4.4 Parameters for $LiNbO_3$

ii. ZnO intermediate and sensing layer



Label: Zinc Oxide

Geometric entity level: Domain

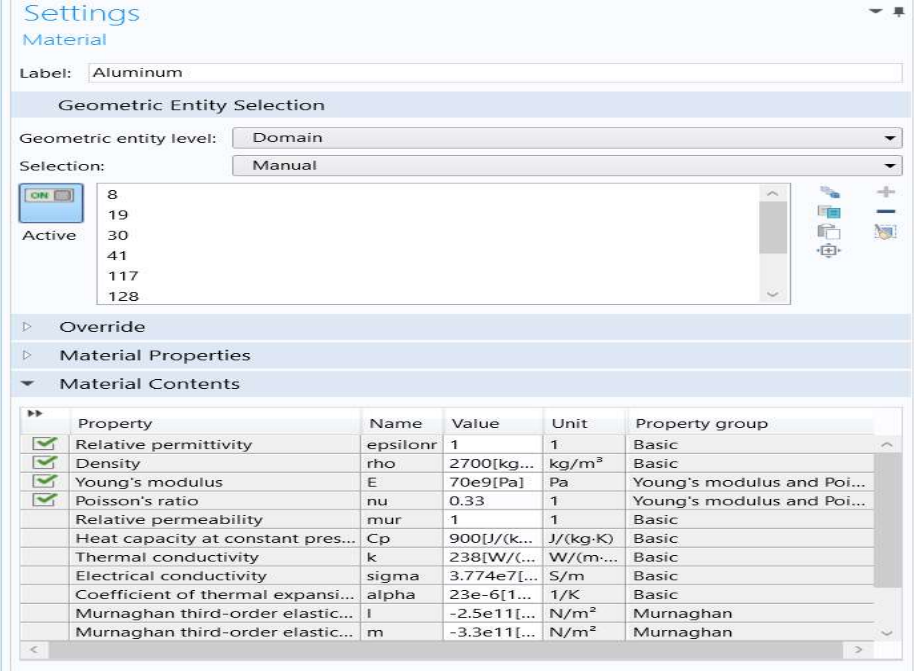
Selection: Manual

2
3
4
5
6
7

	Property	Name	Value	Unit	Property group
☑	Relative permittivity	epsilonr	{8.5446,...	1	Basic
☑	Density	rho	5680[kg...	kg/m³	Basic
☑	Young's modulus	E	2.1e11	Pa	Basic
☑	Poisson's ratio	nu	0.33	1	Basic
	Compliance matrix (ordering:...	sE	{7.86e-0...	1/Pa	Strain-charge form
	Coupling matrix (ordering: xx,...	dET	{0[C/N],...	C/N	Strain-charge form
	Relative permittivity	epsilo...	{9.16, 9....	1	Strain-charge form
	Loss factor for compliance ma...	eta_sE	0	1	Strain-charge form
	Loss factor for coupling matri...	eta_dET	{0, 0, 0,...	1	Strain-charge form
	Loss factor for electrical perm...	eta_e...	0	1	Strain-charge form
	Elasticity matrix (Ordering: xx,...	cE	{2.09714...	Pa	Stress-charge form
	Coupling matrix	eES	{0[C/m^...	C/m²	Stress-charge form

Figure 4.5 Parameters for ZnO

iii. IDTs (aluminium)



Label: Aluminum

Geometric entity level: Domain

Selection: Manual

8
19
30
41
117
128

	Property	Name	Value	Unit	Property group
☑	Relative permittivity	epsilonr	1	1	Basic
☑	Density	rho	2700[kg...	kg/m³	Basic
☑	Young's modulus	E	70e9[Pa]	Pa	Young's modulus and Poi...
☑	Poisson's ratio	nu	0.33	1	Young's modulus and Poi...
	Relative permeability	mur	1	1	Basic
	Heat capacity at constant pres...	Cp	900[J/(k...	J/(kg·K)	Basic
	Thermal conductivity	k	238[W/(...	W/(m·...	Basic
	Electrical conductivity	sigma	3.774e7[...	S/m	Basic
	Coefficient of thermal expansi...	alpha	23e-6[1...	1/K	Basic
	Murnaghan third-order elastic...	l	-2.5e11[...	N/m²	Murnaghan
	Murnaghan third-order elastic...	m	-3.3e11[...	N/m²	Murnaghan

Figure 4.6 Parameters for Aluminium

Boundary setting

There are two types of boundary conditions namely mechanical boundary conditions and electrical boundary conditions. The outer boundaries of the mechanical boundary conditions are set to free condition but the boundary Γ_1 is made to be fixed constraint. While for the electrical boundary conditions, the exterior boundaries are set to zero charge. Now to provide the inputs, 1ST and 3rd electrode of input IDT is given 5V of electrical potential while 2nd and 4th electrodes are kept at ground or default potential. The side boundaries are set to periodic boundary conditions. Boundary conditions for the device are shown in the figure below and are also given in the table given below.

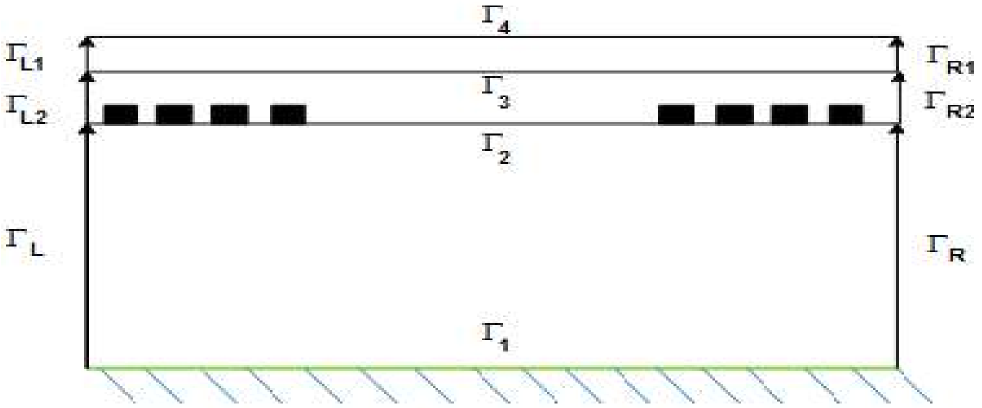


Figure 4.7 Boundary conditions of the sensor

Table 4.2 Simulation boundary conditions

	Mechanical BC	Electrical BC
Γ_1	Free	Zero charge/symmetry
Γ_2	Free	Zero charge/symmetry, Continuity
Γ_3	Free	Continuity
Γ_4	Fixed	Zero charge/symmetry
$\Gamma_L, \Gamma_{L1}, \Gamma_{L2}, \Gamma_R, \Gamma_{R1}, \Gamma_{R2}$	Periodical boundary conditions	

Mesh setting

Meshing process is done to get the nodal representation of the geometry. Meshing can be done in two ways: ‘Physics controlled’ and ‘User controlled’. Former is selected by default and is straightforward. In this the attributes required for tetrahedral mesh for 3D models and triangular mesh of 2D are determined automatically. The user can only change the minimum element size which also is generated automatically and cannot be determined beforehand. Latter is used when the geometry is very complex. For this we use physics controlled mesh and ‘finer’ option for element size.

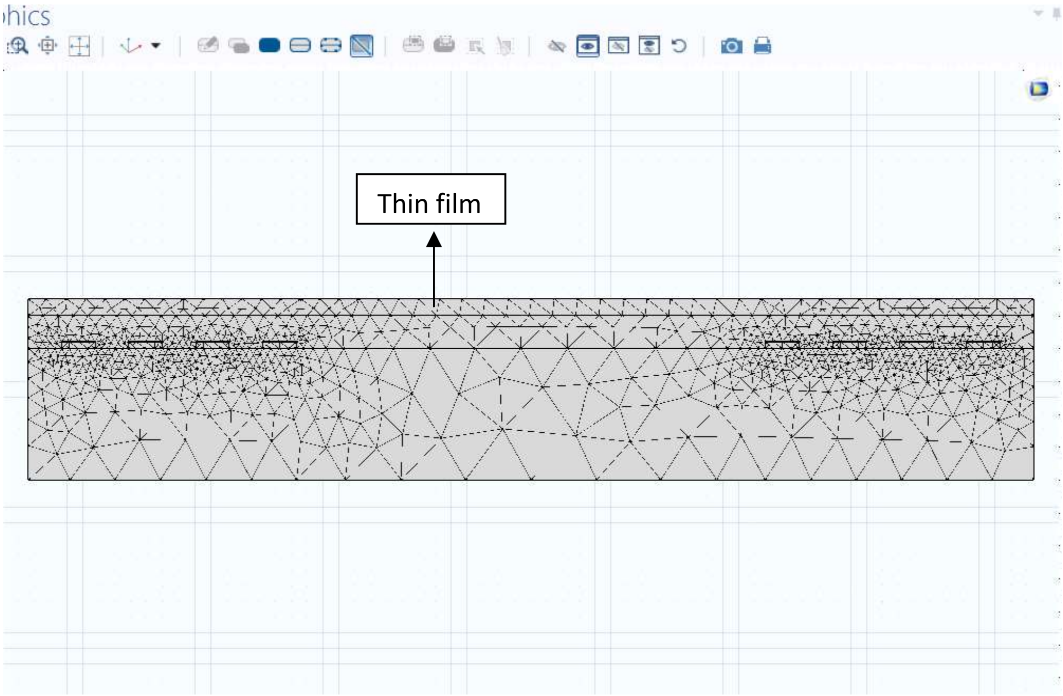


Figure 4.8 Mesh model of the sensor (using thin film)

Study setting

Now this is the final step before getting the simulation results. For our model we will execute eigenfrequency study first to get the optimum electrode height. A parametric sweep is carried out by varying the electrode height from 50 nm to 300nm by using 50 nm as the step size. Then use different materials for IDTs to compare results and get the best one. Then we carry out the time dependent study. The simulation time is set at 0.1 s and the step time is set at 0.001 s. We get total displacement and voltage contour after simulation as output.

4.3.2 2D Structure using nanorods

For this structure we use only time dependent study. This structure has effectively the same dimensions as the layered structure, just that in place of thin film sensing layer, nanorods are used as sensing layer. The meshed structure is shown below, rest of the settings are same as used in the layered design.

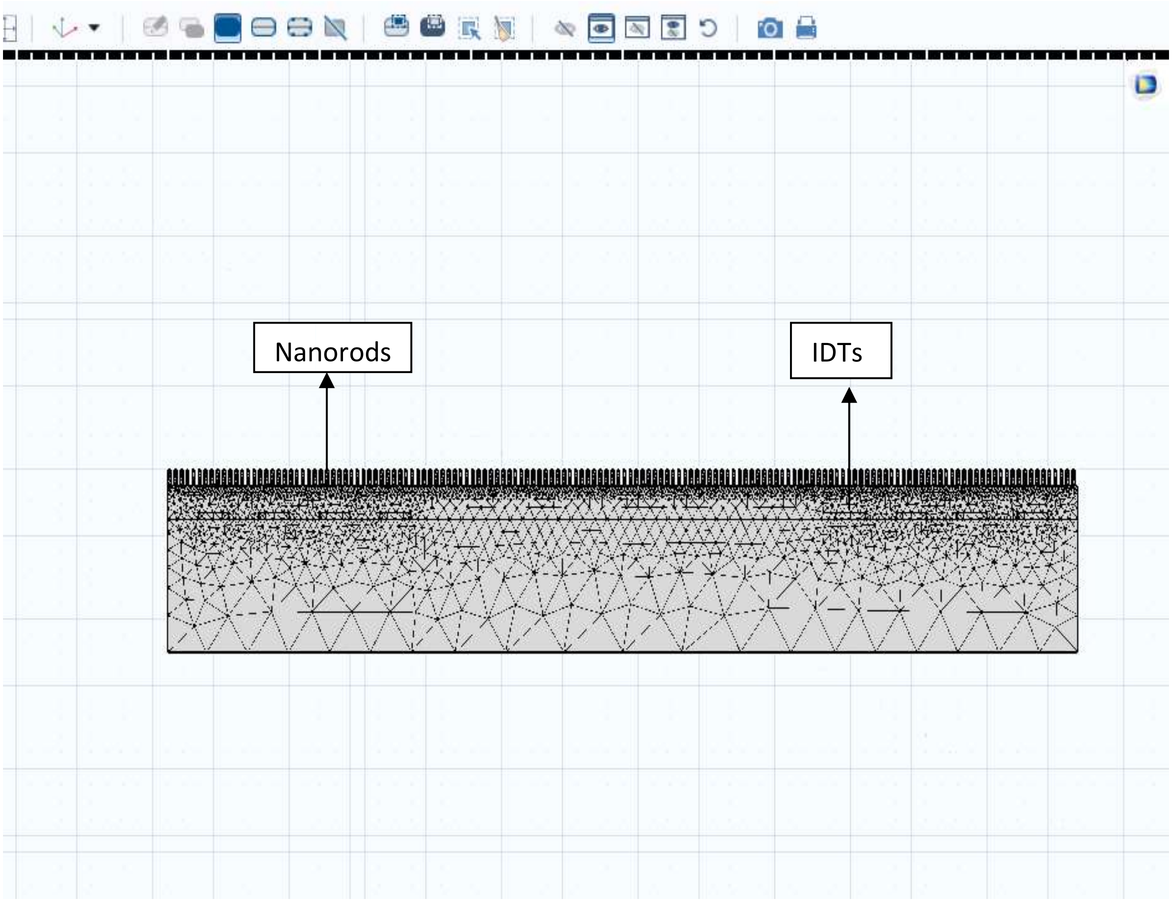


Figure 4.9 Mesh Model of the sensor (using nanorods)

4.3.3 3D structure using nanorods

For this structure we need to select 3D in space dimensions. The dimensions of the substrate are 30µm*10µm*4µm in x, y and z axis respectively. The dimensions of the intermediate layer are 30µm*10µm*1µm in x, y and z axis respectively. The nanorods used in sensing layer are cylindrical. Its radius is 0.1 µm and height is 0.5µm. The dimensions of IDTs are 1µm*10µm*0.2µm. The initial parameters required are same as that used in 2D structures, so same parameters will be used in this. The different settings used in 2D structure are used in this too. Only the geometry of the sensor changes. The geometry and mesh patterns are shown below.

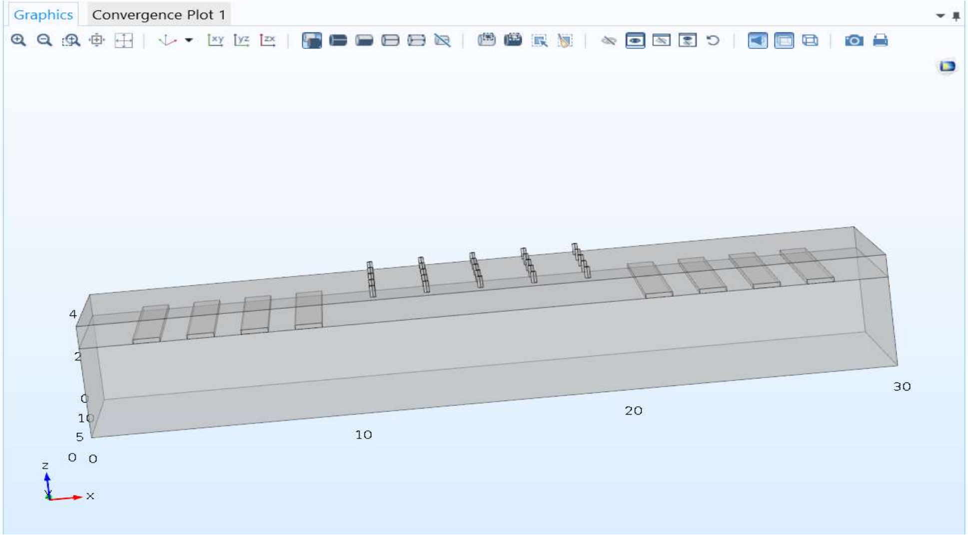


Figure 4.10 3D SAW based gas sensor with nanorods as sensing material

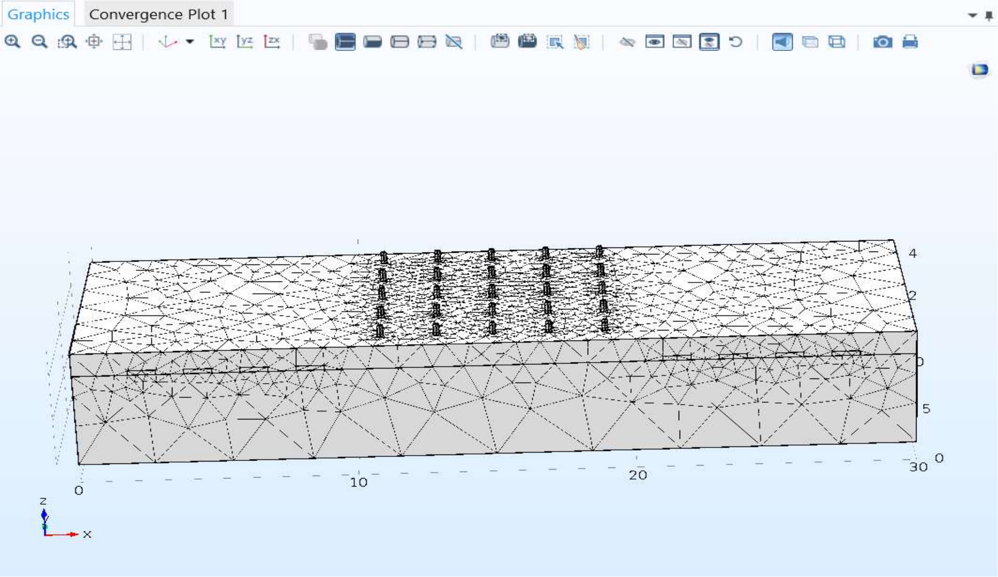


Figure 4.11 Mesh model of the sensor

Transient analysis or Time dependent study is used in this too with simulation time of 0.1s and step time of 0.001s. Then the intermediate layer width is varied using parametric sweep to find the optimum width of intermediate layer.

CHAPTER 5

RESULTS AND DISCUSSION

In this chapter various results of the present study are discussed.

5.1 Optimization of electrode thickness

As for the present study, one of our prime objectives is to find out the optimum thickness for the electrodes of IDT's. Simulations are performed and parametric sweep is used to optimize and compare the results at different electrode thicknesses which will enable us choose an optimum thickness for the best results. The results of the study are presented below:

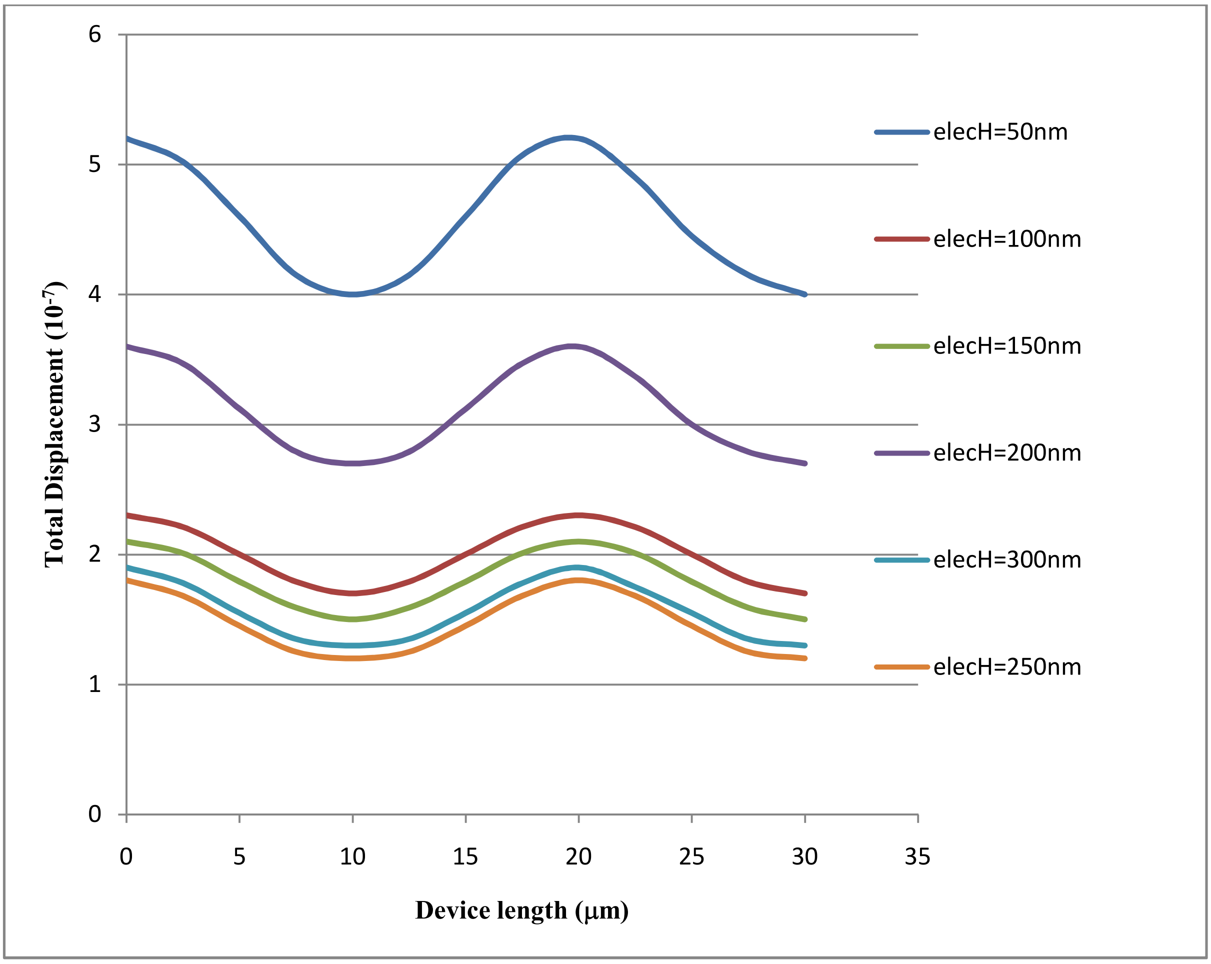


Figure 5.1 Comparison between different electrode thickness

Figure 5.1 shows that highest displacement is when the electrode thickness is 50 nm. But practically, due to fabrication limitations, this much thin layer is not viable. It will be transparent and it could very easily be abraded and in some cases totally removed. Hence it could be concluded the fabrication of 50nm electrodes thickness is not feasible. Now, the next highest displacement is at electrode thickness of 200 nm. Hence, this thickness will be used for the remaining simulations.

5.2 Optimization IDT material

There are various available materials that could be used for making IDTs. In this study, three materials that are widely used as IDTs, namely aluminium, copper and gold, are tested. The simulation results for these materials are shown below:

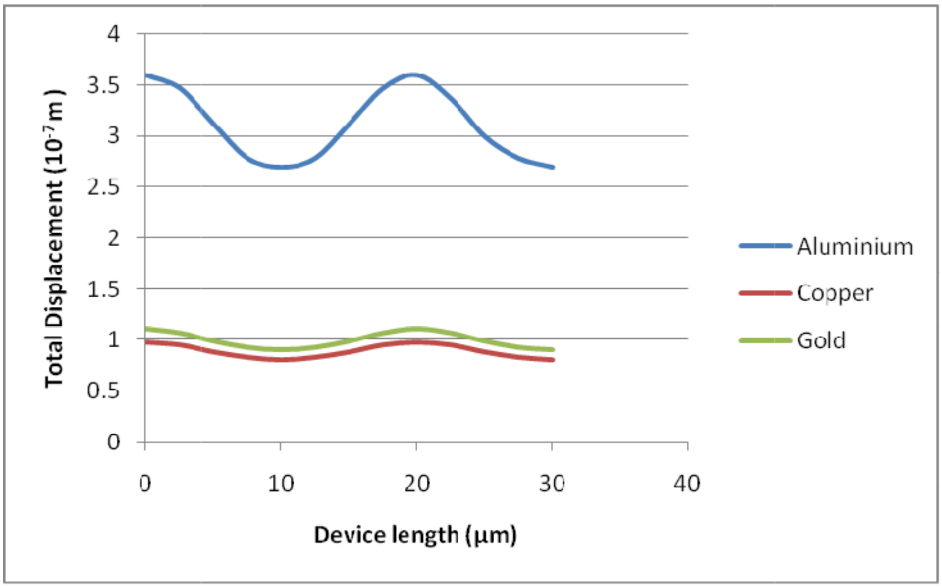


Figure 5.2 Comparison of different materials for IDTs

From figure 5.2, it is clear that aluminium provides much better results than other two materials. The other two materials i.e copper and gold have comparable results and copper shows marginally better results than gold.

5.3 Voltage contour of the sensor

The following simulation is carried out to present the simulation of voltage contour after the sensor is exposed to H_2 gas. A layer of bound charge is produced when the sensor is exposed to H_2 gas, this resulted in production of electric potential and voltage contour.

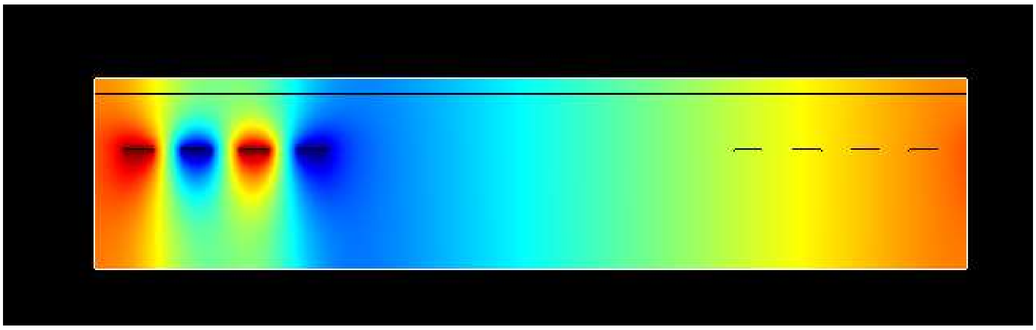


Figure 5.3 Simulation result of voltage contour

The presence of electrical potential within the layer can be observed by different colours in the simulation result. The red colour is observed as higher value while blue presents minimum or zero value. The above simulation shows the energy conversion at the input terminals, the wave has higher potential as represented by red colour. This electrical energy is then converted to mechanical wave as represented by blue colour in the middle of the sensor, as mechanical wave doesn't have any potential. Now, again at the output IDTs, the mechanical wave is converted back to electrical energy as seen in the simulation results.

5.4 Comparison of different architectures of intermediate and sensing layer

In the present work, two different geometries as sensing layer are simulated, one using ZnO thin film and other using ZnO nanorods for sensing H_2 gas. Meshing and simulation of the models has been done to simulate the results. Figure 5.4 and figure 5.5 represents the simulation results as well as a comparison between the two geometries for different intermediate layer thickness.

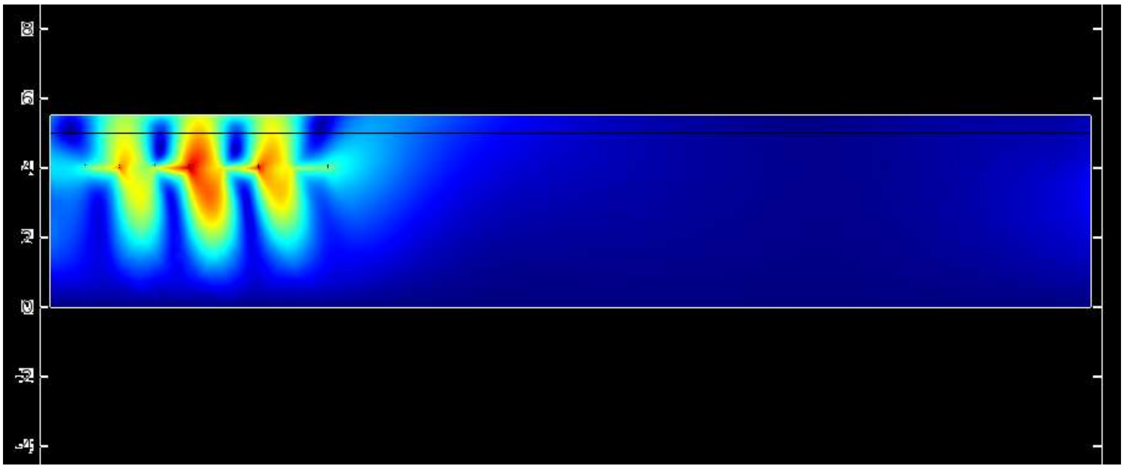


Figure 5.4 Simulation result of 1 µm thick intermediate layer (ZnO thin film as sensing layer)

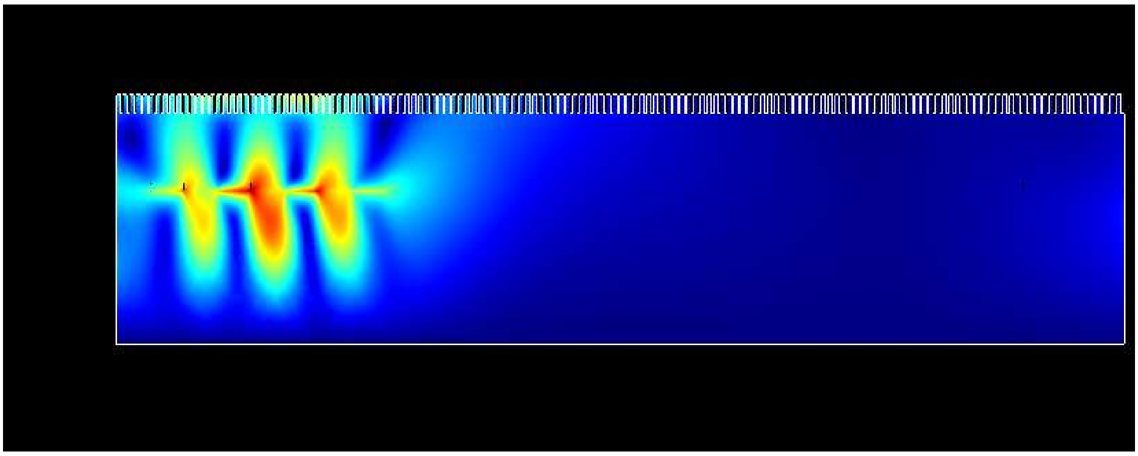


Figure 5.5 Simulation result of 1 µm thick intermediate layer (Nanorods as sensing layer)

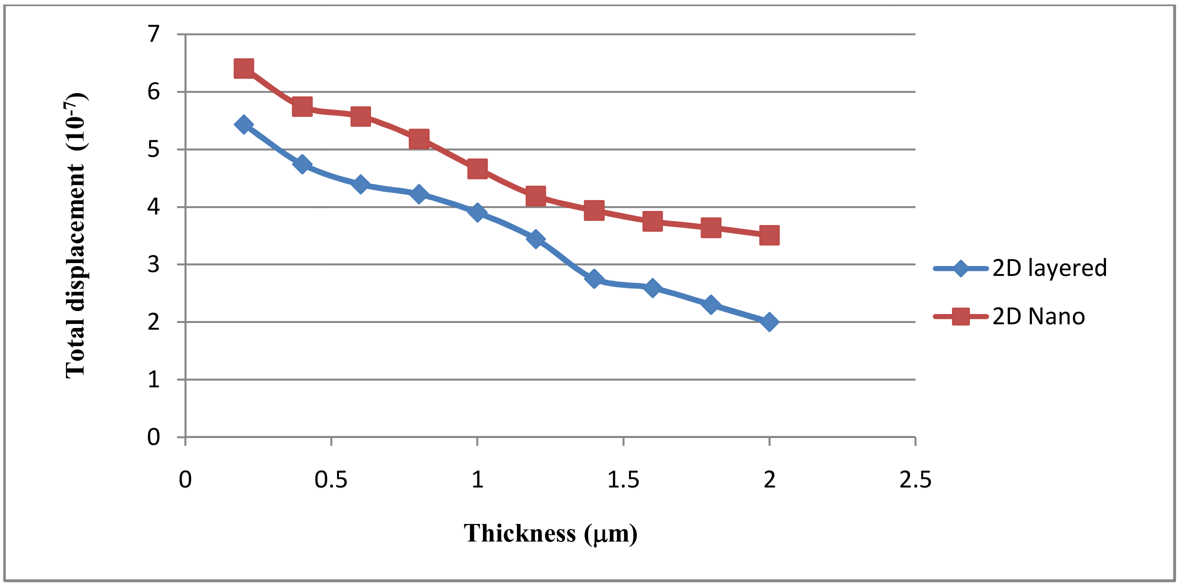


Figure 5.6 Comparison of thin film and nanorods as sensing layer

The comparison shown in figure 5.6 represents that the results with nanorods as sensing material provides better results i.e better sensitivity since displacement is higher. This will be primarily due to high surface area to volume ratio of nanorods as compared to thin film.

5.5 Optimization of thickness of intermediate layer

The sensor is simulated with different widths of intermediate layer. The study presents results with 10 different thicknesses 0.2 μm to 2 μm with a step increase of 0.2 μm. The simulation and displacement results with the sensor exposed to H_2 gas are shown below.

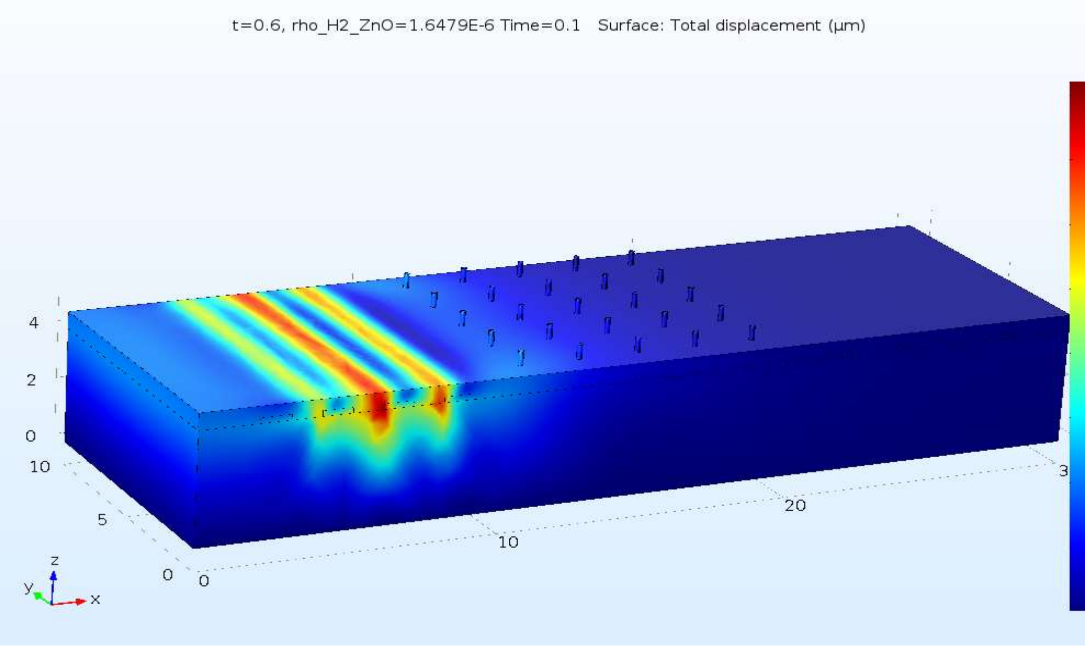


Figure 5.7 Simulation result at 0.6 μm thick intermediate layer after being exposed to H_2 gas

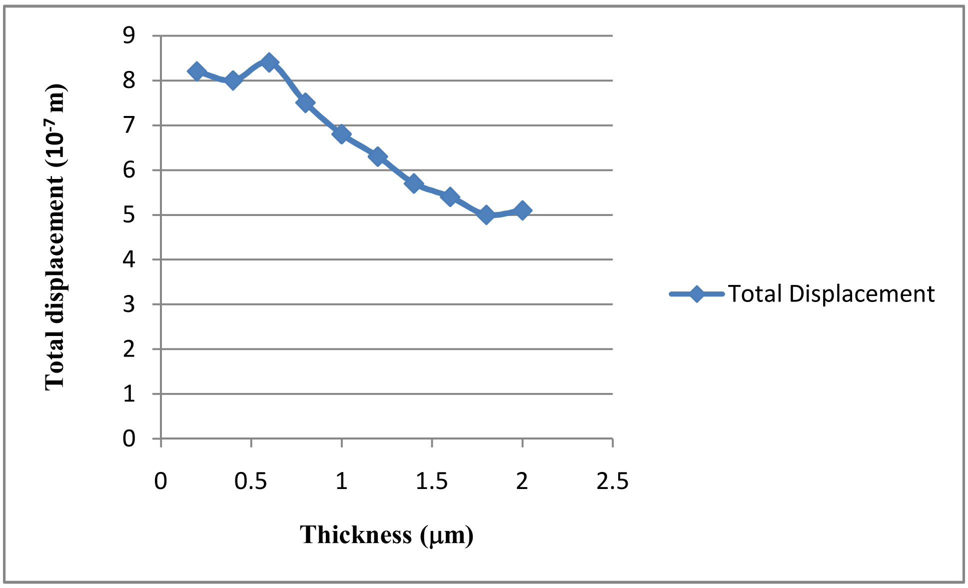


Figure 5.8 Plot of displacement at different intermediate thickness

As shown by the graph presented in figure 5.8, the optimized thickness comes out to be 0.6 μm as it represents the highest displacement value which leads to better sensitivity for the gas sensor. Hence we can conclude that thickness of 0.6 μm of intermediate layer with previously optimized height of nanorods [42] will be an optimized solution for the SAW based H_2 gas sensor.

CHAPTER 6

SENSOR FABRICATION

In this chapter the various steps required to fabricate the sensor are given in detail. The various processes involved and the different tools required to fabricate the device are also explained.

6.1 Fabrication steps

The fabrication process is started using standard techniques. These techniques are followed by thermal evaporation, photolithography, sputtering and at last chemical etching. The various fabrication steps are elaborated as follows:

Sample cleaning

The cleaning process is carried out in class-1000 clean room facility. The 3 inch $LiNbO_3$ substrate is first rinsed with Trichloroethylene (TCE). Then the substrate is ultrasonicated in acetone for about 30 minutes. Then the sample is rinsed with Isopropyl Alcohol (IPA) for 5 minutes. Finally compressed nitrogen is blown over the sample to make it dry.

Substrate metallization

A predopsited Aluminium (Al) over on $LiNbO_3$ is used as substrate. Thermal evaporation technique is used for metallization process with various parameters as follows:

Pressure: 5.1E-6 Torr
Current: 20 Ampere
Deposition rate (Å/sec): 3.2
Thickness: 200nm
Time taken: 11 minutes approximately

Now, the wafer is cut into smaller rectangular samples.

Photolithography

The photolithographic masks are designed and fabricated to make IDT design patterns over the samples of the substrate. The masks are designed and fabricated using high resolution printer over PMMA (Polymethyl methacrylate) thick films [43].

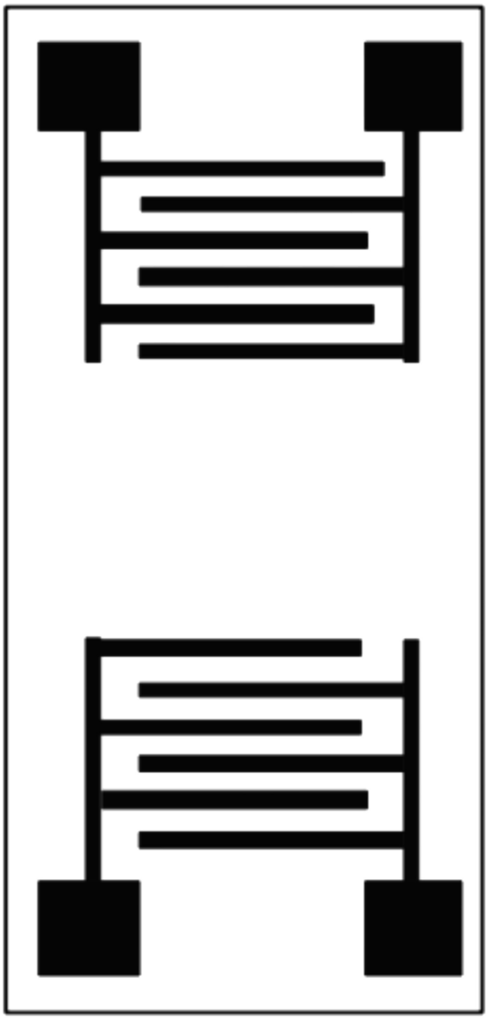


Figure 6.1 Layout of the mask

Then the process of photolithography is carried out using UV photolithography technique. Photolithography is a process by which the designs on the mask are transferred to the metal layer over the substrate. The temperature is maintained at around 21° C and relative humidity of about 35%.

Now for photolithography process, a thin film of positive photoresist S1818 is deposited on the surface of the sample. A positive photoresist is the one which when exposed to UV light becomes soluble. The deposition is done by using a spin coater. Parameters are as follows:

Spin speed: 2500 RPM (revolutions per minute)
Time: 20 seconds
Thickness: Approximately 0.3 µm

Figure 6.2 Spin coater used for depositing photoresist

After spin coating of the photoresist, the sample is soft baked. In soft baking, the sample is heated at about 75° C for 25 minutes using a hot plate. This process will harden the photoresist and a cured film is formed.

Figure 6.3 Hot plate used for soft baking

Then this cured film is exposed to ultra violet (UV) light. This UV light sources has a wavelength of 550 nm. The exposure time is kept between 25 seconds and 32 seconds. After this, the samples are developed using KOH solution (8%) as developer solution. The developing time is about 7-8 seconds and after developing it, the sample is washed with DI (Deionised) water to remove any developer solution.

Figure 6.4 UV exposure unit used for exposing the sample to UV light

Chemical etching

Now, wet etching is used to remove the metallised regions of the sample which are not required. The timing of etching is very critical. Over or under etching could lead to differences in electrode finger widths and this could distort the electrical characteristics of the device.

For etching we use two different ways. One way is to heat the etchant to 45° C and then the sample is immersed in that etchant. The composition of etchant is 80 ml H_3PO_4, 5 ml HNO_3, 5 ml of acetic acid and 10 ml of DI water. Constant stirring is required to prevent formation of bubbles on the sample's surface. The bubbles regress the etching and various under-etched regions may remain. Another way of etching is to use diluted KOH developer which results in even etching of aluminium without the need of stirring. A time period of 2-3 minutes is required to etch a 200nm layer.

Deposition of intermediate layer

To deposit the intermediate layer of ZnO on the $LiNbO_3$ substrate, sol-gel method is used where parameters used are as follows:

Molarity of the solution: 0.3 M

Spin coating: 1500 RPM

Prebaking: at 200°C for 20 minutes
Number of coatings: 4
Annealing: at 550° C for 2 hours

Deposition of sensing layer

ZnO nanorods are used as sensing layer in the gas sensor. To deposit these on the intermediate layer of ZnO we used thermal decomposition process. To synthesise ZnO nanorods, Zn^{II} amino complex is used [44]. An equimolar (10mM) aqueous solution of zinc acetate dihydrate ($Zn(O_2CCH_3)_2(H_2O)_2$) and methanolamine (MEA) are filled in laboratory glass bottles. Nanostructured ZnO thin films are also kept in the bottle and the solution is heated to about 90° C on a hot plate for several hours. Then the ZnO thin films are washed with DI water to remove any remaining salts. Finally well-alligned crystalline nanorods were obtained.

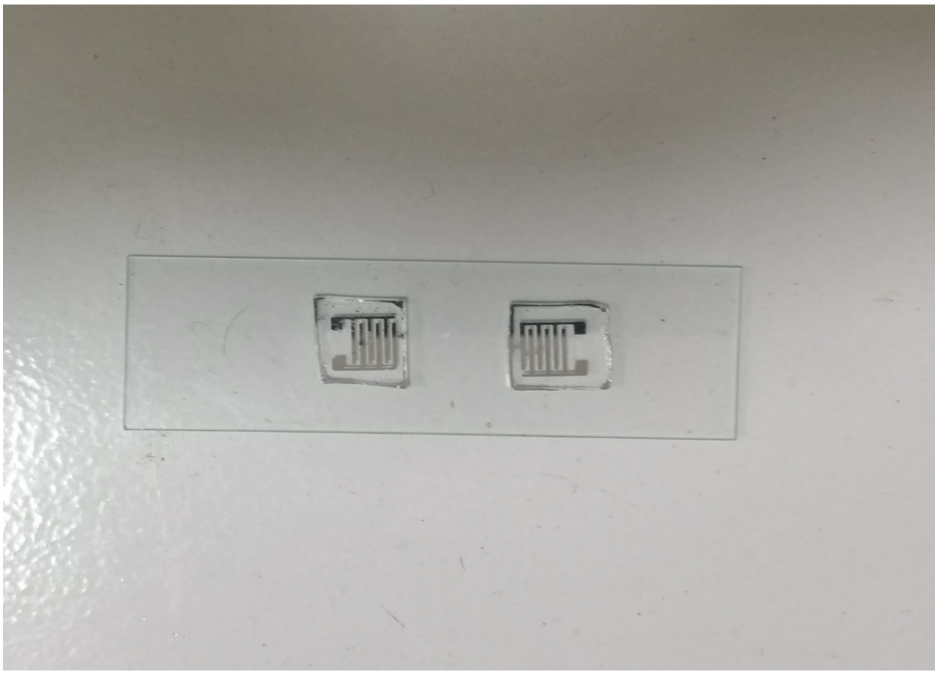


Figure 6.5 Fabricated gas sensor

CHAPTER 7

CONCLUSION AND FUTURE SCOPE

7.1 Conclusion

In the present thesis work, several SAW based gas sensors with different design parameters are studied and simulated. Basically two different structures are studied and analyzed. All these gas sensors are designed to sense H_2 gas and the behaviour of the sensors is studied in presence of gas. COMSOL MULTIPHYSICS 5.2 software is used to design and simulate all these gas sensors.

Various electrode thicknesses are simulated and keeping in mind the practical design constraints 200 nm is selected to be the optimum height. Various materials are also tested to be used as IDT materials but aluminium outperformed others significantly. Then the layer structured with ZnO thin films as sensing layer and layer structured with ZnO nanorods as sensing layer are compared. The structure with nanorods provides better results, mainly due to its high surface area to volume ratio of sensing layer and hence possessing sensitivity. 3D structure is simulated to find the optimum thickness of intermediate layer. The optimum thickness of the ZnO intermediate layer is found out to be 0.6 μm.

7.2 Future Scope

In this study the intermediate layer thickness is varied to optimize the gas sensor. For future works, the sensing layer thickness could also be varied to study the effects on sensitivity. Also different nanostructures could be used in place of nanorods such as nanowires, nanocomb, nanoring etc.

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