Abstract - Low power consuming and high responsive Microelectromechanical systems (MEMS) gas sensors are used for real time environmental monitoring applications. In this paper, a hydrogen gas sensor is designed and simulated using Comsol Multiphysics tool. Gas sensor consists of a micro-heater and a sensing layer above it. A virtual gas environment has been given to the sensor by designing a chamber around the device. The designed sensor is investigated for its response towards hydrogen gas. The resulted change in resistance of the sensor in presence of hydrogen gas is observed.

I. INTRODUCTION

Gas sensors are widely used in many fields such as in environmental monitoring, domestic safety and public security. Even small leakage of some toxic gases may be dangerous to health and life of human being. Hydrogen is considered as one of the best promising source for use in combustion engines and fuel cells as it can be extracted from many available sources. By-products of hydrogen energy are only heat and water vapour which are free from any contamination and can be converted back in to hydrogen and oxygen. Liquid hydrogen is vastly used as a rocket fuel. Due to these benefits, hydrogen powered applications are developed extensively. However, safety issues in the development of hydrogen energy are of a major concern. Hydrogen is the lightest of elements and the smallest molecule; therefore it has the great tendency to leak. It is known to be a colourless, explosive and odourless gas that cannot be detected by human senses. It can be ignited with a very small amount of energy as small as 0.02mJ. The explosive range of hydrogen is wide from 4% to 75%.[1]. Therefore accurate hydrogen detection is necessary considering it explosive properties and its wide range of applications. Metal oxide gas sensor uses the properties of surface adsorption to detect the changes in the properties of the sensing layer [2]. It has been known that the conductance of the sensor varies with the composition of the surrounding gas. An optimal temperature is needed for surface reactions to take place at the upper sensing layer and that temperature is provided by the micro-heater in the sensor device. In this paper, a virtual environment is provided to the sensor by making a gas chamber around the device with the aim of observing surface reactions between the sensor and the surrounding hydrogen gas and then observing the change in the properties of the sensing layer. The design and simulation has been done in COMSOL Multiphysics 5.2.

II. DEVICE STRUCTURE

It has always been a challenge to select proper material for various layers of sensor device. For the present study, polysilicon heater has been used as it consumes the least displacement to achieve the desired temperature, high resistivity, and is also compatible with micromachining processes which make it suitable as a heater material [3]. The major design goal of micro-heater is to maximize the overall thermal efficiency and to attain the uniform temperature distribution throughout the layer. To elevate the temperature of the sensing layer for proper detection of gases, structure shown in figure 1 has been used which consists of silicon dioxide substrate on which poly-silicon heater is placed. Above it there are two poly-silicon inter-digitated electrodes to detect the resistance change in the uppermost tin oxide sensing layer. A single Meander geometry covering area 200 µm X 200 µm of thickness 5 µm has been designed as shown in figure-1. Properties of poly-Si heater used in simulation are given in table 1[4].
Figure 1 3D Model of sensor designed

Figure 2 Interdigitated electrodes placed Coplanar to micro-heater.

Table 1: Properties of poly-Si heater [4]

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coefficient of thermal expansion</td>
<td>2.6e-6[1/K]</td>
</tr>
<tr>
<td>Heat capacity at constant pressure</td>
<td>678[J/(kg*K)]</td>
</tr>
<tr>
<td>Relative permittivity</td>
<td>4.5</td>
</tr>
<tr>
<td>Density</td>
<td>2320[kg/m^3]</td>
</tr>
<tr>
<td>Thermal Conductivity</td>
<td>3.4[W/(m*K)]</td>
</tr>
<tr>
<td>Young’s modulus</td>
<td>160e9[Pa]</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>0.22</td>
</tr>
</tbody>
</table>

III. GAS SENSING MECHANISM

Semiconductor metal oxides possess high surface reactivity and high sensitivity of electro-physical properties to the gas phase composition. More specifically zinc oxide and tin oxide are known for their good sensitivity and selectivity towards various gases. Operating temperature of the sensor is carefully monitored so that sensor senses a particular gas as each gas responds at a different operating temperature. SnO₂ is a metal oxide which shows high sensitivity towards reducing gases such as hydrogen [5]. When metal oxide is exposed to air, the oxygen molecules absorbed on the surface change to oxygen ions by gaining electrons from the conduction band of SnO₂, and when it is exposed to reducing gas (like hydrogen), the gas molecules are oxidized by the oxygen ions on the sensor surface which results in the release of free electrons to the metal oxide and consequently, there is an increase in the conductance of the layer as given in equation 1, 2, 3 respectively.

\[ O^{2-} + 2e^{-} \rightarrow 2O^{-} \]  \hspace{1cm} (1)

\[ H_2 \rightarrow H + H \] \hspace{1cm} (2)

\[ 2H^+O^- \rightarrow H_2O + e^- \] \hspace{1cm} (3)

IV. SIMULATED RESULTS

A gas chamber of 1mm height and 1mm diameter with 0.05 mm radius of inlet as shown in figure 3 is designed around the sensor device which is filled with the hydrogen gas. Concentration of gas in the chamber is varied with the time so that it can be recorded that how resistance of layer is varying with time.

Figure 3 Gas chamber

Figure 4 shows the result after applying simulation with the designed characteristics, that when the concentration of hydrogen gas has been varied from 1 mol/m³ to 50 mol/m³, sensing layer shows a decrease in resistance, proving that sensor device designed is changing its properties on the introduction of the gas as the hydrogen being a reducing gas, resistance of layer must decrease as proved through these simulated results. Figure 5 is the input concentration pulses of the gas varying w.r.t. time that has been introduced in the chamber during simulation. Various concentration pulses are given over time to ensure the gas sensing mechanism. Figure 6 shows its corresponding
result that how resistance changes after gas injection and purge [6].

Figure 4 Comparison of resistance of layer as a function of varying concentration of gas.

Figure 5 Input concentration pulses

Figure 6 Dynamic response of sensor to input concentration pulses of figure 5

Figure 7 Plot between Resistance of layer w.r.t heater voltages

Figure 8 Comparison of normalised sensor response magnitude for different gas concentrations vs operational temperature.

V. CONCLUSION

This study has demonstrated a mems based gas sensor, featuring a tin oxide sensing layer. Sensor device is tested for its changed electro-thermal properties under controlled environment. It was seen that sensor exhibited an increase in the
conductance on exposure to hydrogen gas at different concentrations and operating temperatures. It has been also found that by varying the operating voltage of heater, reaction rate between gas and layer can be controlled and the optimal temperature at which the sensor gave the maximum response was found to be around 450K and because of increased reaction rate, the reaction time decreased, correspondingly the response time of sensor gave an evident decrease.

VI. REFERENCES


