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Design and Optimization of a Microheater for the Application of Indium Tin Oxide (ITO) based Gas Sensor in VOC Detection

Chayanika Sharma
Instrumentation & USIC,
Gauhati University,
Gauhati- 781014, Assam, India
chayanika114@gmail.com

Utpal Sarma
Instrumentation & USIC,
Gauhati University,
Gauhati- 781014, Assam, India
utpal.sarma.in@ieee.org

***Abstract*—Microheaters have been extensively investigated for its wide application in designing a Metal Oxide Semiconductor based gas sensor. Indium Tin Oxide (ITO) deposited on a thin glass film can be made use to detect various Volatile Organic Compounds (VOCs) at different elevated temperatures. To achieve this higher temperature requirement, power management is also a very crucial part of gas sensor design. In this paper, four different structures of microheater are discussed. The simulation was carried out using Finite Element Method. The length and structure of the microheater were varied for optimization. From the simulated designs of microheater, the optimized one was calculated by considering two important aspects, power management and uniform temperature distribution over the gas sensitive layer of the gas sensor. Hence this kind of gas sensor design with an inbuilt temperature modulating part shows potential application towards VOC profiling in future work.**

***Index Terms*—ITO, VOC, microheater, MOS**

I. INTRODUCTION

The complex hydrocarbons, present in the gaseous form at normal temperature and pressure are termed as Volatile Organic compounds (VOCs) [1].The impact of the VOCs in the environment we dwell in is very important. These compounds may sometimes cause a significant hazard for humans and animals. VOCs can be termed as one of the major causes of air pollution. The release of a huge amount of these gases are induced by different small-scale industries/laboratories, industrial zones, automobiles, agriculture, and landfills [2].

Apart from different sophisticated analytical techniques such as gas chromatography, spectroscopic systems, etc. some portable miniaturized devices are developed, and used to detect the VOCs present in the environment. Conductometric gas sensors based on Metal Oxide Semiconductor (MOS) are grabbing attention as most promising among the other sensors to estimate the presence of different types of gases. The high sensitivity as well as high selectivity, rapid response time, low power consumption, and low fabrication cost are the key parameters associated with the increasing popularity of these MOS based sensing devices. Despite numerous advantages, MOS based sensors require elevated operating temperatures (typically, 300-750K) for the detection of VOCs. The response of the MOS-based sensors can be improved using some distinct types of catalytic layers and additives to the sensing material. By this process, the selectivity of the material towards the gases to be tested and the operating temperature can be reduced. Furthermore, the reduction of the particle sizes in the sensing layer to nanoscale helps in achieving the optimum response towards the target gas [3][4].

The application of Indium Tin Oxide (ITO) was reported by several researchers for the estimation of occurrence of gases like acetone, methanol, ethanol, CO_2, NO, NO_2, CCl_4, butanol etc. [5][6]. The advantages of using ITO material-based gas sensor are its linearity and excellent stability against temperature variation. Moreover, ITO based sensors can be interfaced with an electronic circuit easily without any complex signal conditioning unit because of the resistivity of the material, which is in the range of $10^{-4}\Omega$ cm to $10^{-5}\Omega cm$ [7][8]. Furthermore, the response of these sensors can be improved by incorporating a catalytic layer at any one surface of the sensing material. Using this method, the disadvantage of elevated temperature requirement by a MOS based gas sensor can be diminished by some amount [9].

Temperature uniformity in the gas sensor is a crucial factor to improve sensitivity as well as selectivity in order to detect certain VOCs. A particular type of sensor design can be made applicable for detection of different gases at a range of elevated temperatures. For example, SnO_2 based sensing material responds to NO_2 in the temperature range of 303353K, while ammonia responds at higher temperature (523573K) [10]. Therefore, the design and optimization of a microheater plays an important role in the gas sensor design [11]. In this paper, an approach to design and optimize a microheater for the optimum response of an ITO based gas sensor is made and discussed.

The structural organization of the paper is as follows: architecture of the gas sensor, computer simulation, simulation results & discussion and conclusion.

TABLE I: Calculated dimensions of the gas sensor for simulation

	Dimension(mm)	Thickness (mm)
Glass substrate	26x26	0.5
Sensing layer	24x24	0.05
Silver electrodes	1.5x1.5	0.03

II. ARCHITECTURE OF THE GAS SENSOR

The gas sensor design proposed in this work comprises of a microheater, electrodes and a MOS based sensing surface deposited on glass substrate as shown in Fig.1. The Finite Element Method is employed to design the structure of the gas sensor. Thin film of indium tin oxide with the resistivity of 70-100 $\Omega/square$, which is deposited on a glass substrate has been chosen as the sensing material for this study. The dimensions of the sensor are given in TABLE I.

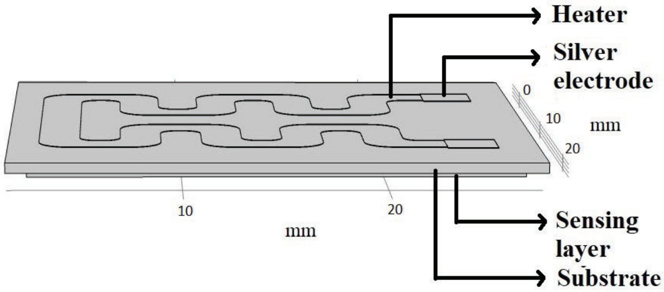

Fig. 1: Gas sensor design

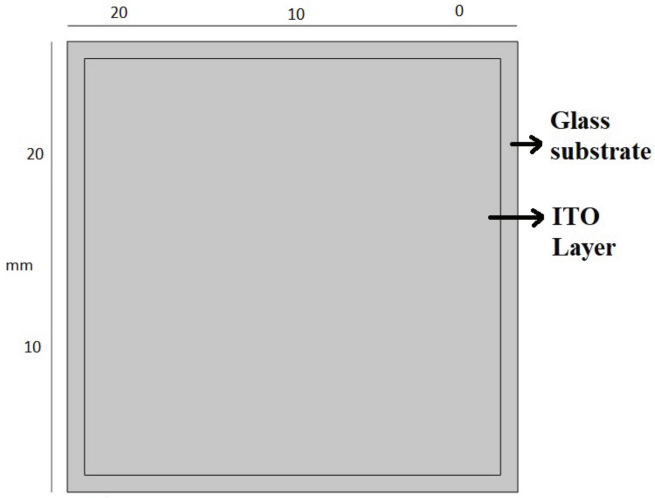

Fig. 2: Sensor design in simulation

A. Microheater

The performance of a microheater based gas sensor depends on the geometries, sizes and the selection of material. These microheaters need to be smaller in size and should consume low power with higher temperature stability at elevated temperature applications. So, material selection is a crucial part in microheater design. In this paper a heater is designed and optimized using nichrome material using Finite element method. The thickness of the heating material is kept at 0.03mm. Two square shaped silver pads of dimension 1.5mmx1.5mm are used as contacts of the heater. The properties of the microheater material used for simulation are given in TABLE II.

III. MATHEMATICAL MODEL AND NUMERICAL SIMULATION

The simulation was performed using Finite Element Method. The modelling and simulation depend on several physical constraints, such as the geometry, the structure & shape of the model, the materials chosen for simulation and the type and size of selected feature mesh. The designed sensor is shown in Fig.2.

A. Physics applied in the mathematical modelling

The computer-based simulation model basically consists of two physics interfaces: electric current and heat transfer in solids. In this study four different types of heater structures were designed and simulated (shown in Fig.3). The dimensions of the designed heaters are given in TABLE III.

The distribution of electric field (E), across the microheater can be defined as follows [12] :

$$E = -\nabla V = -\nabla(I_{in}.R_{heater}) \tag{1}$$

In the above equation, V is the voltage applied at the heater ends. A constant current source (I_{in}) is applied at the both heater contacts. R_{heater} is the resistance of the heating material.

In the physics interface, used for Joule heating, the temperature increases due to the resistive heating of the conductor, which is generated as a result of applied electric current. The resistive heat (Q), generated due to the microheater arrangement is given by the following equation:

$$Q \propto |J|^2 \tag{2}$$

Where, $|J|$ is the magnitude of electric current density.

TABLE II: Properties of the heater material used for simulation

Material Properties*	Values
Thermal conductivity	15(W/(mK))
Density	9000(kg/m^3)
C_P	20(J/(kgK)
σ	9.3x10^5(S/m)
Relative permittivity	1

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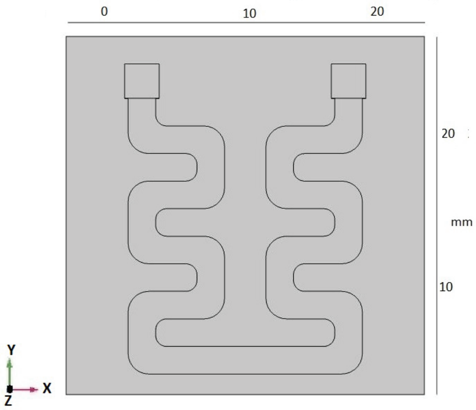
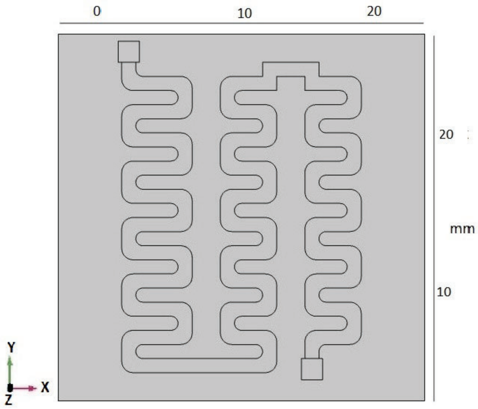
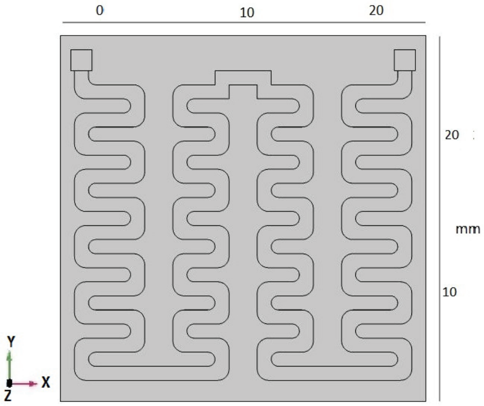
* *Where, C_P and σ are the specific heat capacity and electrical conductivity of the used material, respectively.*



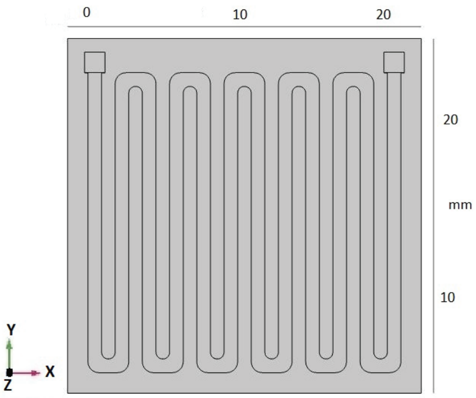
[Heater1]



[Heater2]



[Heater3]



[Heater4]

Fig. 3: Designs of microheater structures in simulation

TABLE III: Dimensions of thr microheaters designed in simulation

	Length (mm)	Resistance (Ω)
Heater1	81.673	1.49
Heater2	170.92	5.84
Heater3	241.05	8.20
Heater4	273.14	9.93

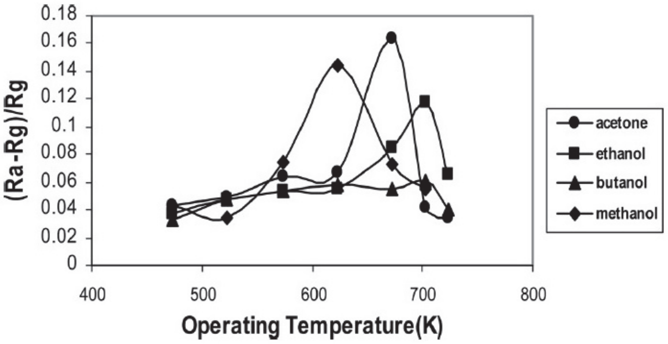


Fig. 4: Response of ITO based gas sensor for different VOCs [7]

Where, R_a and R_g are the resistances of the ITO-based gas sensor at the exposure of air and target gas, respectively.

IV. RESULTS AND DISCUSSION

The stationary study is used to compute the temperature generated due to the resistive heating of the designed heating circuit. Four different heater structures were designed as shown in Fig.3. The temperature generated due to the applied electric current is calculated for each design. V. S. Vaishanv et. al, in 2006 [7] reported the maximum operating temperatures for optimum response of an ITO based gas sensor (as shown in Fig.4) for VOC detection. Present work aims at obtaining the maximum desirable temperature for a very low input power. Fig.5 depicts how temperature changes with respect to the change in input current for different heater structures.

For proper operation of a gas sensor, the temperature disribution over the gas sensitive layer should be uniform. Fig.6-9 shows teperature distribution at different arclengths of the sensing layer for the designed heater structures. For heater1, the temperature distribution (shown in Fig.6) is gradually decreasing along the length of the sensing layer, which is not desirable. Fig.7 shows the temperature distribution curve for heater2. From this curve, it can be inferred that the slope of the temperature distribution curve with respect to different arclengths of the sensing layer is decreased from the previous one. The same plot for heater3 is shown in Fig.8. The slope of this curve is very small. For heater4, the temperature distribution plot (shown in Fig.9) is almost linear, which is a desirable condition to enhance the selectivity of the gas sensor for a particular VOC. The Y-axis labels for the reported four figures (Fig.6-9) are different due to the fact that, the temperatures obtained at different arclengths over the gas sensitive layer for each heater are different at the applied input currents of same value (shown in the legends).

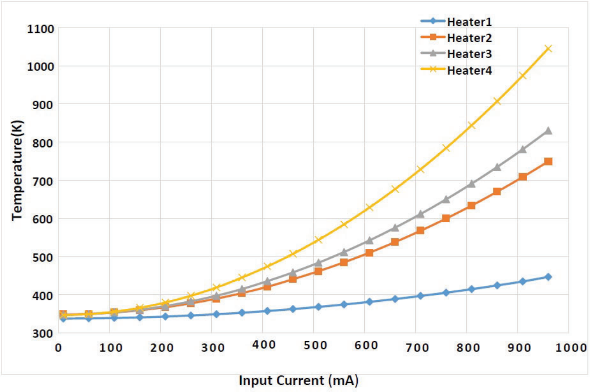


Fig. 5: Temperature generated due to different heater structure

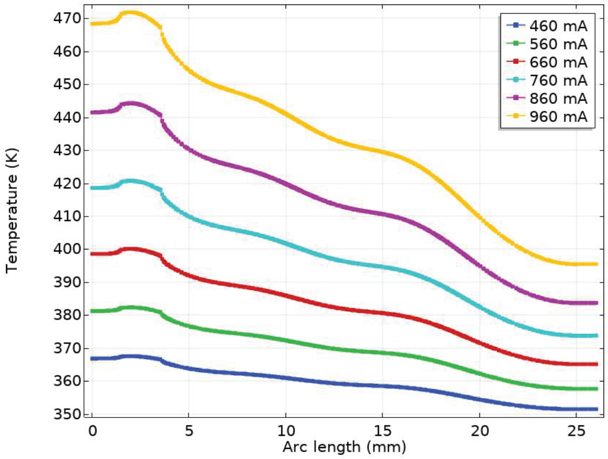


Fig. 6: Temperature at different arc length for heater1

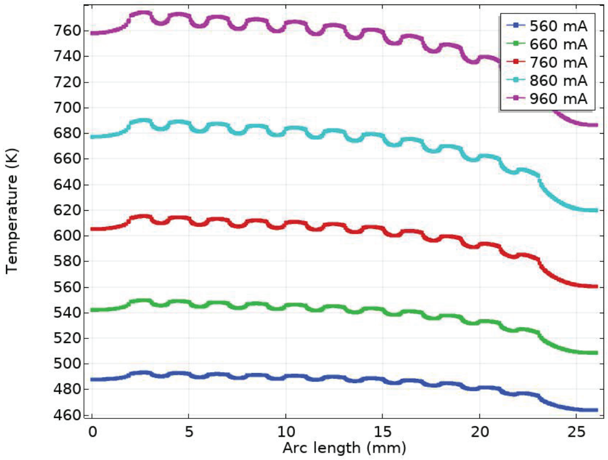


Fig. 7: Temperature at different arc length for heater2

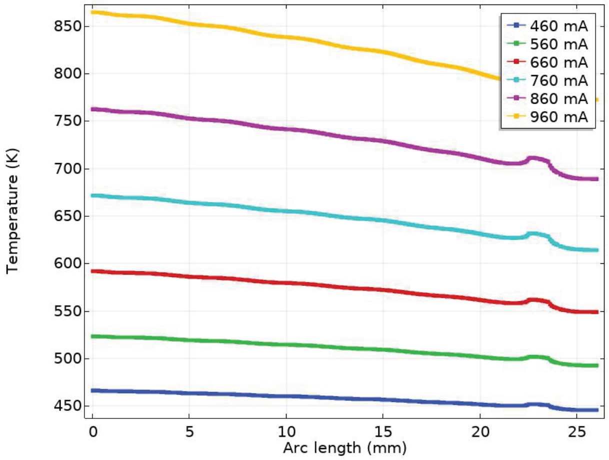


Fig. 8: Temperature at different arc length for heater3

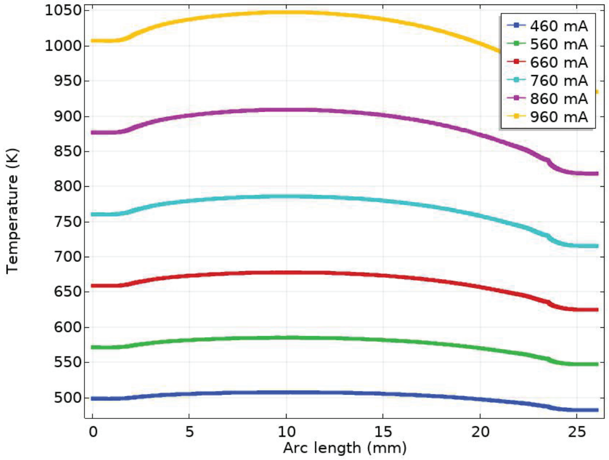


Fig. 9: Temperature at different arc length for heater4

From the simulation results, it can be said that the resistive heat generation due to heater4 reaches the desired level mentioned in Fig.4 at a very low input power. Again, the temperature distribution curve due to heater4 is found to be uniform for different arc lengths of the designed sensor.

V. CONCLUSION AND OUTLOOK

In this work, we successfully designed, simulated and optimized a heater structure to provide the required temperature for a MOS-based gas sensor. In summary, a Finite Element Method model has been developed to simulate different designs of microheater to achieve elevated temperature requirement for gas sensing applications. The heater's length, area and structure was changed in order to obtain the desired outcome. The optimization was done by considering two important factors of gas sensor design: to achieve desired temperature at a lower value of input power, and to get an undeviating temperature distribution across the gas sensitive layer of the sensor. From the results obtained from simulation, it can be seen that the heater4 has all the desired properties, and hence it is best suited for the above-mentioned application.

Overall, it may be said that this design of heater structure with an inbuilt temperature modulating part can be modified for future applications like designing a single MOS based gas sensor for detection of various VOCs at different temperatures.

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