3D Stationary and Temporal Electro-Thermal Simulations of Metal Oxide Gas Sensor based on a High Temperature and Low Power Consumption Micro-Heater Structure using COMSOL TM

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Abstract: We have developed a metal oxide gas sensor based on a micro-heater structure on a membrane able to work until 550°C, with a power consumption equal to 60mW at this temperature. In this paper, we have presented the electro-thermal simulation of this structure with COMSOL™, in order to check the temperature distribution on the surface, compare the maximum temperature between simulation and measurement for different power consumption, find the time necessary to obtain a stabilized temperature. The results obtained are: a good distribution of the temperature at the surface of the structure, the simulated and measured temperature curves in function of the power consumption are very close, the time required to stabilize the temperature of the membrane is about 60ms.

Keywords: Gas sensor, micro-heater, metal oxide, membrane

1. Introduction

The basic principle of gas detection with metal oxide sensors is based on the variation of conductivity of a semi-conductor material, in function of the nature and the concentration of gases in contact with this material. The main advantages of this kind of sensors are: a low cost, very sensitive and fast responses to gases, easily miniaturized. These sensors may be used to detect poisonous gases (CO, NO_2) [1], odorous gases (SO_2, H_2S) [2], flammable gases (CH_4, C_3H_8) [3], …

The main role of the heater resistance is, with a high temperature, to easily desorb the gas molecule in contact with the sensitive layer. This temperature must be at least 400K [4]. The higher the temperature is, the easier the desorption is [5]. But a higher temperature implies a higher power consumption. And in the case of gas sensor, the largest application is for embedded systems, so the power consumption must remain low enough. There is a compromise to find between high temperature and low power consumption [6].

1.1 Micro-heater technological process

For this purpose, we have developed a micro-heater structure with these characteristics. The substrate is silicon. On this substrate, we did grow a bi-layer membrane SiO_2/SiNx. On the membrane, we have deposited the two electrodes (heater and sensitive) by evaporation; the deposited metal is platinum with a bonding layer of titanium. On the metallization layer, we did grow a SiO_2 passivation layer. After that, we have realized the open contact with a chemical etching. To liberate the membrane, we realize a backside RIE (Reactive Ion Etching) to etch the backside membrane deposition, and a DRIE (Deep RIE) to etch the silicon substrate. To finish, we have deposited the sensitive layer by inkjet. In this paper, we will use zinc oxide (ZnO) as sensitive layer. The finished component has dimensions of 2mm*2mm.

2. COMSOL™ Parameters

The results presented in this paper are from COMSOL™ 4.2 version.

2.1 Physics

The physics model used to simulate our work is the Joule Effect model. A first equation defines to electric potential.

$$\boxed{-\Delta.(\sigma.\Delta V) = 0}$$

With: - V the electric potential

Equation 1. Electric potential equation

A second equation describes the heat transfer.

$$Q = \rho . Cp . \frac{dT}{dt} - \Delta . (k . \Delta T)$$

With: - Q the heat source
- ρ the density
- Cp the heat capacity
- k the thermal conductivity

Equation 2. Heat transfer equation

These two equations are linked by a third equation, the Joule Effect equation.

$$Q = \sigma . |\Delta V|^2$$

With: - σ the electrical conductivity

Equation 3. Joule Effect equation

To realize the studies and solve the equations, we have used a MUMPS solver.

To respect the test conditions in our gas system, we have added at the surface of the sensor an inward heat flux equal to 125W/m².

2.2 Electrodes material

The heater and sensitive electrodes are in platinum. The characteristics of the material used are described in the following table.

Parameter	Unit	Value
Thermal Conductivity (k)	W/(m*K)	73
Electrical Conductivity (σ)	S/m	2.94e6
Density (ρ)	kg/m^3	21440
Heat Capacity at Constant Pressure (Cp)	J/(kg*K)	132
Thermal Expansion Coefficient (α)	1/K	8.8e-6
Young Modulus (E)	Pa	150e9
Poisson's Ratio (ν)	1	0.35

Table 1. Material properties of platinum

2.3 Mesh

To mesh correctly the structure, we have tried several possibilities and the best choice was: a free tetrahedral geometry with a geometric scale of 1/1/1 (x/y/z) for the wafer, and a free tetrahedral geometry with a geometric scale of 0.01/0.01/1 (x/y/z) for the rest of the structure.

The selected mesh size is "normal", because the results obtained with this configuration is better than with "coarse" and similar with "fine". The complete mesh consists of 27440 elements.

3. Results

The objective of these simulations is to design a model faithful to our real micro-heater structure to be able to simulate the future evolutions before designing it.

3.1 Temperature distribution

In this first simulation, we have observed the temperature distribution on the surface of the passivation layer without sensitive layer. We have applied a voltage of 5V across the heater resistance, which corresponds to a power consumption of 57mW, deduced from the following equation.

$$P = \frac{V^2}{R}$$

With: - P the power consumption
- R the resistance

Equation 4. Power consumption equation

The results obtained have been presented in 3D (Figure 1) and in 2D (Figure 2), in degrees Celsius.

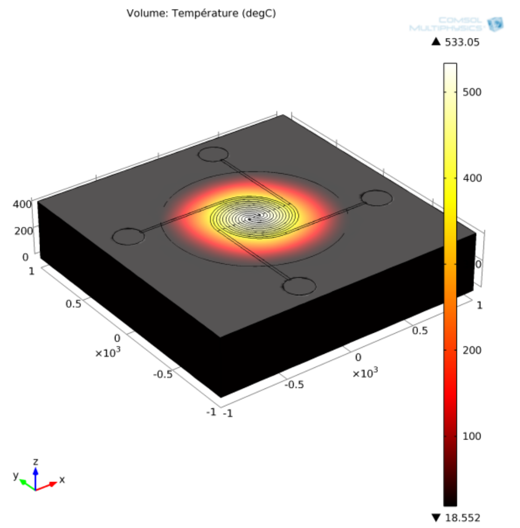

Figure 1. 3D temperature distribution in the gas sensor without sensitive layer – Heater voltage = 5V

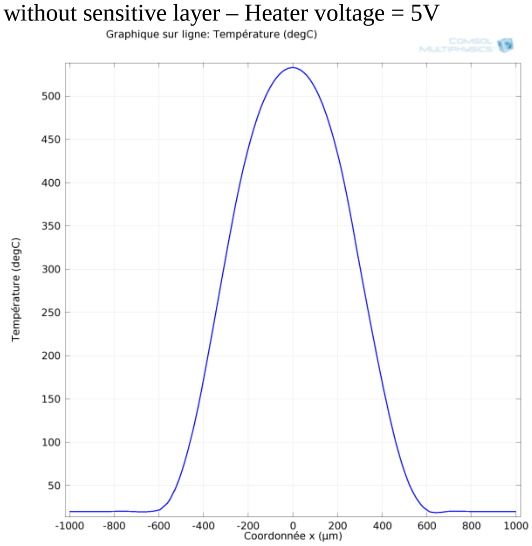

Figure 2. 2D temperature distribution at the surface of the passivation layer – Heater voltage = 5V

The maximum temperature with 5V is 533°C at the center of the surface. The temperature gradient between the center and a circle of diameter 500µm, which corresponds to the limit of our sensitive layer deposition, is around 100°C. Moreover, the maximum size of the open contact is a circle of diameter 340µm, and the temperature gradient with the center is 70°C

3.2 Power consumption

In order to validate the results obtained in the previous section, we have compared the maximum temperature obtained by simulations for different voltages applied across the heater, to infrared measurements with a real sensor (without sensitive layer).

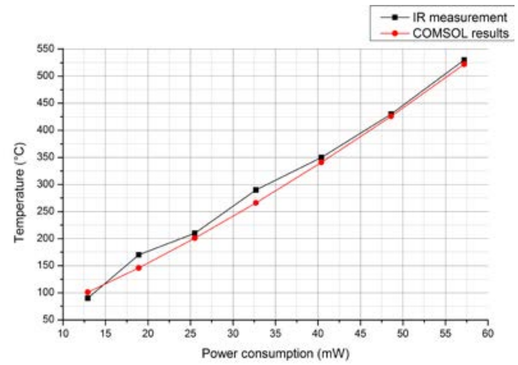

Figure 3. Temperature versus power consumption at the surface of the passivation layer with COMSOL^{TM} simulations and infrared measurement

The two plotted curves are very close and the maximum deviation is below 25°C. This graph is used to validate the modeling of our sensor.

3.3 Influence of the thickness of the sensitive layer on the surface temperature

We have added at the previous design simulated a sensitive layer modeled by a cylinder of 500µm of diameter. The thickness of sensitive layers deposited by our inkjet system is between 0.5µm and 1µm. The material used is ZnO from the library materials. The voltage applied across the sensitive resistance is 0.1mV.

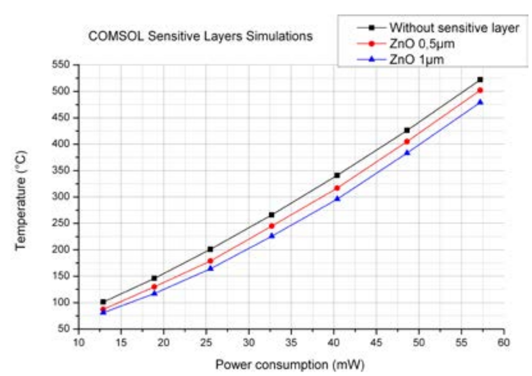

Figure 4. Temperature versus power consumption for different ZnO sensitive layer thickness

For a power consumption between 35mW and 60mW, the difference of the maximum temperature between a structure without sensitive layer and with a 0.5µm layer of ZnO is around 25°C. At the same power consumption range, the difference of the maximum temperature between a structure without sensitive layer and with a 1µm layer of ZnO is around 50°C.

3.4 Temporal temperature stabilization

To simulate the transient voltage, we have replaced the continuous voltage applied across the heater resistance by a transient step between 0 and 5V in 100ns.

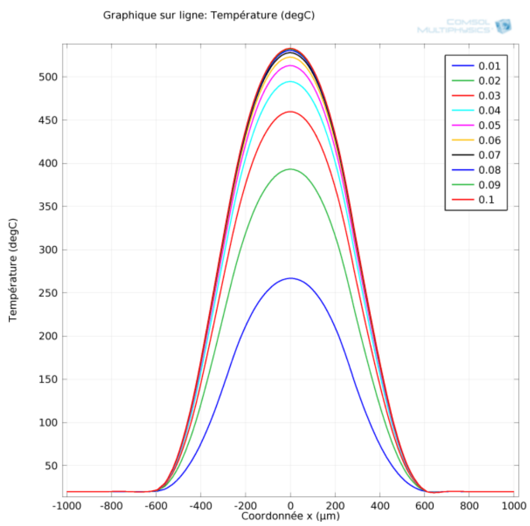

Figure 5. Temporal variations of temperature at the surface of the passivation layer for a heater power from 0 to 5V

We have obtained curves that converge toward the same temperature as in stationary study (533°C) and we can consider that the temperature is stabilized after around 60ms.

4. Conclusions

The purpose of this work was to create a model faithful to our real micro-heater. The simulated results are really close to the measurement. We have successfully modeled our low power and high temperature structure.

In addition, we have observed that the temperature uniformity is suitable for our application, the influence of a sensible layer on the maximal temperature which decreases of 25°C for a 0.5µm ZnO layer at high temperature, and the transient time equal to 60ms when we apply a voltage step from 0 to 5V.

These results are promising and the model created will be helpful for the next optimizations of our structure.

5. References

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