Study on thermal field coupling simulation of methane sensor based on ceramic micro-hot plate

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Abstract: In view of the lack of high concentration online gas detection sensors in the current mine safety monitoring system to cope with gas emission and gas outburst, a design method of full-range gas sensor based on ceramic micro-hot plate is presented in this paper. COMSOL finite element simulation is used to study the thermal field coupling of sensor array units. Based on the electro-thermal coupling model, the thermal field was established, and the influence of isolation groove, base material, working temperature and platinum film thickness on the thermal interference between the sensor units was studied. The results show that the heat loss is reduced by 2.57 times and the heating efficiency is improved. Compared with AlN and SiC ceramic substrates, Al2O3 has the least thermal disturbance and the best thermal performance. The average working temperature at 1.3v reaches 587.77k. The temperature difference between the units is directly proportional to the unit operating temperature. Increasing the thickness of platinum film can improve the working temperature and heating efficiency. The research provides a theoretical basis for the design of the integrated MEMS array gas sensor.

1. Introduction

In recent years, the Al2O3, AlN, SiC and other ceramics have become research hotspots in the field of gas sensor due to their high temperature resistance, easy mass production and integration of multiple working units [1-2]. However, when each element of the array sensor working, the thermal field will be generated around it, and the superimposed coupling of the thermal field will generate thermal interference, which will affect the temperature size, thermal stability and detection accuracy between the sensor units [3]. Zhou Zhen [4] find that thermal interference between cell size on integrated sensor array thermal stability has important significance, based on aluminum nitride ceramic of the micro hot plate under 163 °C heat disturbance test analysis. Zhao Wenjie [3] analyzed the thermal interference of 4 - cell sensor array based on semiconductor principle at 200 °C from the structural
design, demonstrated the influence of structural design on thermal interference between AlN micro-hotplate array cells, isolated the structural design, and reduced the loss of heat conduction. Russian researchers [5] made microheaters and electrodes on the 10-30um aluminum oxide film obtained by spark oxidation, and fixed the film structure on the pre-microfabricated aluminum oxide ceramic base, and found that the heat loss was significantly reduced.

The above researches show that thermal isolation design is an indispensable part of the sensor array. In view of the lack of high-concentration on-line gas detection sensors in the current mine safety monitoring system to deal with gas gushing and outburst, a design method of full-range gas sensor based on ceramic micro-hotplate is proposed by integrating catalytic combustion and thermal conductivity into multiple working units of array sensors and using the compensation unit in the catalytic system as the sensitive unit of thermal conductivity system. Therefore, it is necessary to study the thermal interference of multi-working units of the sensor under high temperature (above 400 °C), so as to provide a reference for the design of the integrated full-range methane sensor.

2. Full range methane sensor structure
The integrated full-range methane sensor is composed of three functionally independent heating units integrated on the same ceramic substrate. The heating units have a completely symmetrical distribution structure. as shown in fig. 1a, the catalytic sensing unit, the catalytic compensation unit (and the thermal conductivity sensing unit) and the thermal conductivity compensation unit are sequentially arranged from left to right [6]. Pads are provided at both ends of the electrode for soldering Pt leads. The chip structure is designed to be square with a substrate thickness of 100 μm; The bow electrode is made of Pt silver paste, with a thickness of 10-20μm, a resistance wire length of 15.63 mm, a cross-sectional area of 50μm×63μm, and a static resistance of 6.94Ω at normal temperature. The lead material is Pt wire with purity of 99.9 %. The maximum cell size of model grid generation is 5.5x10⁻⁴, and the minimum cell size is 4x10⁻⁵. The overall structure and grid generation of the chip are shown in figure 1.

3. Numerical simulation conditions

3.1. Heat conduction model
The thermal field simulation analysis of the chip is realized by Comsol directly coupling of the electro-thermalphysical field [7]. The calculation formula of electric-thermal physical field is as follows:
The current continuity equation represents the distribution of the potential on the conductor in the model after the voltage is input to the model, and its formula is:

$$\nabla [\sigma(T) \nabla U(\vec{r}, t)] = 0, \quad U|_{\Gamma_d} = \bar{U}(t), \quad \frac{\partial U}{\partial n}|_{\Gamma_q} = -\frac{j(\vec{r}, t)}{\sigma(T)}|_{\Gamma_q}.$$  

(1)

Where: $T$ temperature is a function of space and time, $\vec{r}$ representing a space vector and $T$ representing time. $\Gamma_d$ is the boundary where the first type of boundary condition is located and $\Gamma_q$ is the boundary where the second type of boundary condition is located. $\sigma(T)$ is the conductivity of the material varying with temperature, which will also become a function of space and time, and $U(\vec{r}, t)$ is the transient spatial potential field distribution. $\bar{U}(t)$ is the voltage value on. $j(\vec{r}, t)$ is the current density distribution.

The heat conduction equation represents the temperature distribution of heat conduction on the micro-thermal plate, and the expression is as follows:

$$\rho c \frac{\partial T(\vec{r}, t)}{\partial t} + \nabla[k(T)\nabla T(\vec{r}, t)] = f^T(\vec{r}, T, t), \quad T|_{\Gamma_d} = \bar{T}, \quad \frac{\partial T}{\partial n}|_{\Gamma_q} = -h(T - T_a)|_{\Gamma_q}.$$  

(2)

In the formula, $k(t)$ is the temperature-dependent thermal conductivity of the material, which is also a function of space and time, and $c$ and $\rho$ are the heat capacity and density of the material, respectively. $T(\vec{r}, T)$ transient spatial temperature field distribution. $f^T(\vec{r}, T, t)$ is a transient space heat source, which will include the sum of Joule heat and other heat sources of the energized conductor. $\bar{T}(T)$ is the temperature value on the first type boundary $\Gamma_d$; $H$ is the thermal convection coefficient on the second boundary $\Gamma_q$; $T_a$ is the ambient temperature on the convection surface; $N$ is the outer normal direction of the boundary $\Gamma_q$.

### 3.2. Comparison scheme and simulation hypothesis

According to the structural design method of the ceramic micro-hotplate array methane sensor, considering the influence of isolation tank, carrier material, working temperature and other factors on its thermal field.

Thermal analysis of chips is based on the heat balance equation which includes three heat transfer modes of heat conduction, thermal convection and thermal radiation. The applied physical field includes three parts: Joule heating, heat transfer and solid mechanics. Model boundary conditions refer to the reference [2]. The main parameters of materials in the model are shown in table 1.
Table 1. Material properties

| Attribute | \( \lambda \) (W/(m·K)) | C/J.(K)\(^{-1} \) | \( \rho \) (g/cm\(^3\)) | Thermal expansion coefficient \(^{\circ}\text{C} \times 10^6\) | E/(Pa)\(^{9}\) | \( \sigma \) (S/m)\(^{-6}\) | \( \mu \) |
|-----------|------------------|-----------------|----------------|-----------------------------|-------------|-----------------|--------|
| Pt        | 71.6             | 133             | 21450           | 8.80                        | 168         | 8.9             | 0.38   |
| \( \gamma \)-Al\(_2\)O\(_3\) | 30               | 730             | 3965            | 7.7                         | 400         | 0               | 0.22   |
| AlN       | 200              | 710             | 3260            | 4.5                         | 340         | 0               | 0.25   |
| \( \alpha \)-SiC | 180              | 800             | 3200            | 4.4                         | 41          | 0               | 0.14   |

4. Simulation results and analysis

4.1. Analysis of thermal interference effect of isolation groove on heating unit

The input voltages of the three units are all set to 1.3V, and other physical parameters refer to the chip structure description. COMSOL software simulated the temperature distribution cloud picture in the case of setting the isolation tank and without the isolation tank, and set the temperature calculation path L, as shown in Figures 2.

Figure 2. Temperature contrast of micro-hot plate

Figure 2 shows the maximum heating center temperature 587 K, the substrate temperature 550 K, and the temperature difference 37 °C; The maximum heating center temperature of the isolation tank is 628.54 K, the substrate temperature is 548 K, and the temperature difference is 80.5 °C. The latter is 43.5 °C higher than the former. The temperature of the two substrates is similar. It reflects that the existence of the isolation groove increases the temperature of the heating unit, reduces the heat loss and improves the heating efficiency.

After analysis, the setting of the isolation groove is to replace Al\(_2\)O\(_3\) with air in the heat transfer path, which greatly reduces the heat transfer performance, reduces the heat loss due to heat transfer, and improves the heating efficiency. According to the thermal conductivity equation, the heat loss of the micro-hotplate without isolation groove was calculated to be 508 MW. Since the overall heat transfer area is almost unchanged, the operating voltage of the micro-hotplate with isolation groove is changed to make the temperature difference the same as that without isolation, resulting in a heat transfer loss of 227.4 mW and a loss reduction of 2.57 times.

4.2. Analysis of influence of substrate material on thermal interference of heating unit

Different ceramic materials have different material properties, which will affect their heating efficiency. Under the conditions of voltage of 1.3 V and film thickness of 10 μm, the sensor thermal field distribution of ceramic materials Al\(_2\)O\(_3\), AlN and sic as base materials was simulated, respectively, as shown in figure 3.
Figure 3 shows the highest temperature 628.54 k, the lowest temperature 547 k and the temperature difference 81.54 k on the Al$_2$O$_3$ micro-thermal plate. The highest temperature on SiC micro-hot plate is 518 K, the lowest temperature is 477.7 K, and the temperature difference is 40.3 K; AlN has a maximum temperature of 440.7 K, a minimum temperature of 419.3 K, and a temperature difference of 21.4 K.

Figure 3. Temperature comparison of different substrates along path L

Compared with the three materials, the thermal efficiency is Al$_2$O$_3$ > SiC > AlN. The thermal conductivity of the material is positively related to the thermal conductivity. As Al$_2$O$_3$ has the smallest thermal conductivity and the least heat loss, using Al$_2$O$_3$ as the substrate in the design will effectively reduce thermal interference.

4.3. Analysis of influence of operating temperature on thermal interference of heating unit

With Al$_2$O$_3$ as the base material, the platinum film thickness was set to 10 $\mu$m, and the operating voltages were controlled from 0.9v to 1.4 v with step of 0.1v. Simulation results are shown in fig. 4.

Figure 4. Temperature distribution under different voltage of sensor

Figure 4 shows that the voltage increases from 0.9v to 1.4v, The average temperature of the micro heating plate is 435, 469, 506, 546, 587.75 and 638.1k; The temperature difference of the substrate is 39, 49, 59, 70, 81 , 96 K, respectively. According to calculation, the ratio of temperature difference to the average temperature of the substrate is 9%, 10%, 11%, 12%, 13% and 15% in sequence. The linear correlation coefficient between the temperature difference of the substrate and the average temperature of the substrate is 0.9944. The temperature difference of the substrate is proportional to the average operating temperature of the substrate. The higher the operating temperature of the substrate, the smaller the relative thermal interference.

Since the change of platinum film thickness and the change of input voltage directly affect the resistance value of heating resistor and thus the temperature distribution. With Al$_2$O$_3$ as the base material, the working voltage was set to 1.3 v, and thermal field simulations were carried out for platinum film thickness of 10 $\mu$m, 20 $\mu$m and 30 $\mu$m, respectively, as shown in figure 5.
Figure 5 shows that the substrate temperature differences corresponding to the three cases of platinum film thickness 10, 20 and 30 μm are 81.5, 157.8 and 227.5 k respectively. As the heating resistance decreases with the increase of platinum film thickness, the operating temperature increases, the temperature difference increases, and the relative thermal interference decreases.

5. Conclusion

Through COMSOL simulation research, the following conclusions are drawn:

(1) If there is a temperature difference between the units, thermal interference will exist. Thermal isolation design concentrates the high temperature distribution inside the isolation tank structurally, reducing thermal interference and improving heating efficiency. Therefore, isolation tank can be set in the production of full-range methane sensor.

(2) The degree of thermal interference is also different with different substrate materials. In this study, Al₂O₃ is the best substrate for reducing thermal interference and has the highest thermal efficiency. Therefore, Al₂O₃ is selected as the substrate material for the full range methane sensor.

(3) Increasing the thickness of the platinum film from 10 μm to 30 μm will increase the working temperature, which will lead to a larger temperature difference of the substrate and a reduced degree of thermal interference. At the same time, with the increase of the working voltage, the working temperature of the substrate increases and the relative thermal interference decreases. Therefore, in the actual production of full-range methane sensor, according to the actual situation, with reference to this rule, the platinum film thickness is appropriately adjusted. Better selection of operating voltage during operation.

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