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Temperature distribution on dielectric membrane structures for sensitive elements of semiconductor gas sensors

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Abstract. The aim of this article is to show a simulation of temperature distribution on dielectric membrane structures with membranes of different dielectric materials in the measuring mode of a semiconductor gas sensor. The simulation results were obtained using the software package Synopsys TCAD. In various moments of the measuring cycle were obtained two-dimensional temperature distributions on membrane structures. Dependencies of temperature versus time for the variety of the coordinates on membranes, temperature versus coordinates at the sensitive layer area's highest heat value and temperature versus time in the center of the membranes are presented. Recommendations are given for the selection of membrane material for the heat-insulating membrane structure of sensitive elements for semiconductor gas sensors.

1. Introduction

In modern trends of MEMS technology development, due to the constant miniaturization of MEMS elements, the process of their design becomes increasingly complex and at this time cannot be efficiently implemented using existing analytical methods. Therefore, recently, in order to obtain high-quality results and reduce the time of design, computer-aided design is increasingly used. Modern simulations capabilities allow to visually demonstrate to a high degree of accuracy the final characteristics of the device under development and the processes occurring in them. It contributes to the optimization of material selection for device realization and technological modes of its production [1-3].

In recent times, for the analysis of gaseous environments are increasingly used semiconductor gas sensors [4, 5]. The measurement of gas concentration for such sensors requires the pre-heating of sensitive layers. It selectively accelerates the processes occurring on the surface and in the volume of the sensitive layers. Thereby, the selectivity of semiconductor gas sensors is provided for [6-10]. The possibility of achieving a high temperature of the sensitive layers is mainly influenced by heat exchange in the surrounding environment through the construction of sensitive elements. A distinctive design feature of such sensitive elements is the presence of a heat-insulating structure [11, 12]. The most promising heat-insulating structures for sensitive elements of semiconductor gas sensors are dielectric membrane structures. (Such a structure is shown in Fig. 1.) This is explained by that dielectric films have the lowest coefficient of thermal conductivity among all known materials [13, 14]. However, the formation of sensitive layers on such membrane structures is complicated by the fragility of dielectric membranes [15-17]. It requires the formation of sensitive layers exclusively before the formation of the



membranes. The authors of this article have developed a new method to create sensitive elements based on dielectric membrane structures [18-21]. The main distinction of this method is that it involves the formation of membranes after the formation of the sensitive layers [22, 23].

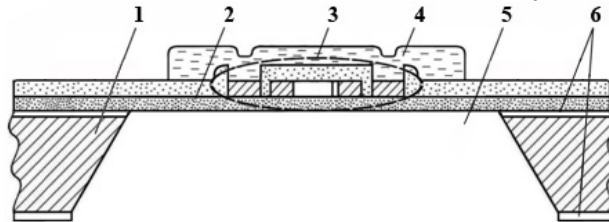


Figure 1. Structure of the sensitive element on the dielectric membrane: 1 – silicon substrate; 2 – dielectric membrane; 3 – structural elements (resistive heater, resistive temperature sensor, sensitive layer contact area); 4 – sensitive layer; 5 – cavity under the membrane; 6 – thermal silicon oxide layer.

The selection of the optimal dielectric membrane material is necessary to provide the required temperature conditions of gas concentration measurement and for the development of this new technology of sensitive elements for semiconductor gas sensors based on dielectric membrane structures. For this purpose, knowledge of temperature distribution on membranes of different dielectric membrane structures in measuring mode of the semiconductor gas sensor is required. In this article, the results of the simulation of the temperature distributions on dielectric membrane structures in the semiconductor gas sensor's measuring mode are shown, and were obtained using the software package Synopsys TCAD.

2. Simulation

The dielectric membrane structures are to be implemented on substrates of monocrystalline silicon of orientation (100), with a diameter of 76 mm and thickness of $(380 \pm 20) \mu\text{m}$. The thickness of the membranes is to be about $1\text{--}3 \mu\text{m}$.

For the simulation was built a model of the membrane structure with a platinum resistive heater in the center of the membrane, presented in Fig. 2. The thickness of the substrate was adopted to $10 \mu\text{m}$. This was done because the actual substrate thickness ($380 \mu\text{m}$) sharply increases the simulation time, while not significantly affecting the results of the final simulation. The membrane size taken was equal to $1 \times 1 \text{ mm}^2$. The thickness of the membrane was chosen to be $2 \mu\text{m}$. The strip width of the resistive heater was made as $20 \mu\text{m}$, the strip length was taken at 2.95 mm and the strip thickness adopted was $0.5 \mu\text{m}$. The area of the heating region was calculated at about 0.3 mm^2 . Calculated resistance of the heater at room temperature was about 31.5Ω . The simulation of temperature distribution was carried out by the application to the resistive heater of a rectangular pulse with voltage level equal to 1 V and duration 100 ms . Rise time and fall time of the pulse amounted to about 10 ms each. The total time of simulation for the cycle of heating and cooling (measuring cycle) was equal to 210 ms .

The simulation of temperature distribution was carried out on membrane structures with membranes of silicon oxide, silicon nitride and silicon oxynitride. Since the simulation of composite compounds in the software package Synopsys TCAD is not provided for, silicon oxynitride membrane was modeled as a four-layer membrane. It was modeled with alternating layers of silicon oxide and silicon nitride with a thickness of $0.5 \mu\text{m}$ each. The properties of this membrane are close to that of silicon oxynitride membrane.

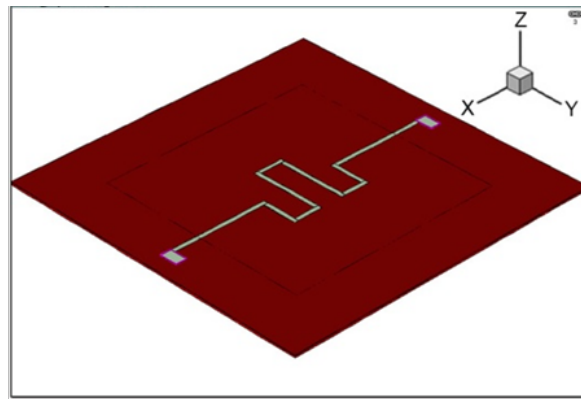


Figure 2. Model of the membrane structure (with a coordinate system that has zero in the center of the membrane).

For all membrane structures, at the application of the rectangular pulse on the resistive heater at various moments of the measuring cycle were obtained two-dimensional temperature distributions, presented in Fig. 3-5. Also, for all the membrane structures were obtained the dependencies of temperature versus time for the measuring cycle of a variety of coordinates on membranes, presented in Fig. 6-11. Besides, for all the membrane structures were obtained dependencies of temperature versus coordinates (with zero in the center of the membranes) at the moment of the highest heat for the sensitive layer area and with temperature versus time for the center of membranes, presented in Fig. 12, 13.

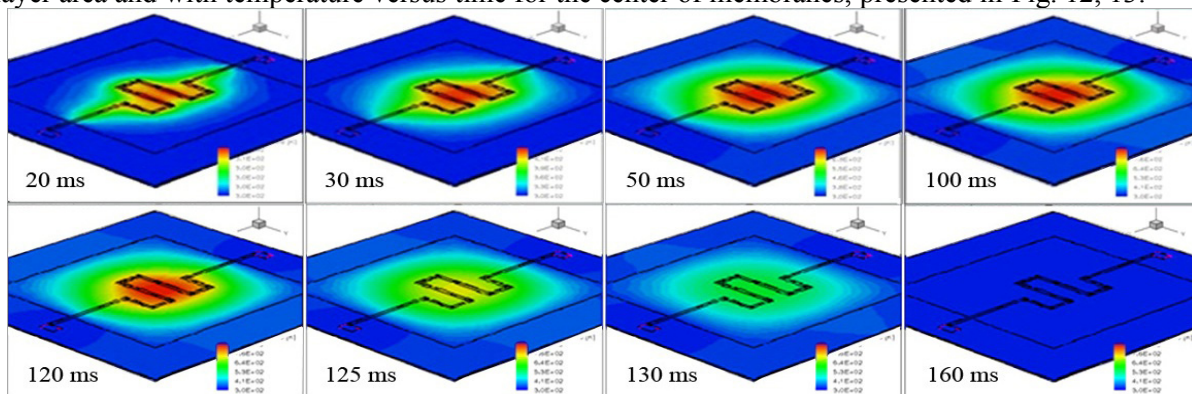


Figure 3. Two-dimensional temperature distribution on the silicon nitride membrane.

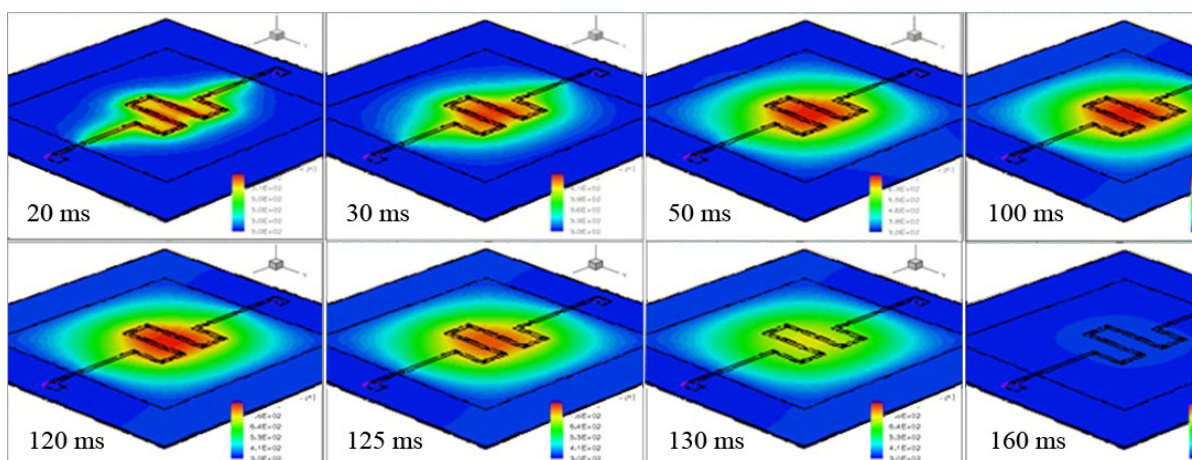


Figure 4. Two-dimensional temperature distribution on the four-layer membrane (close to the silicon oxynitride membrane).

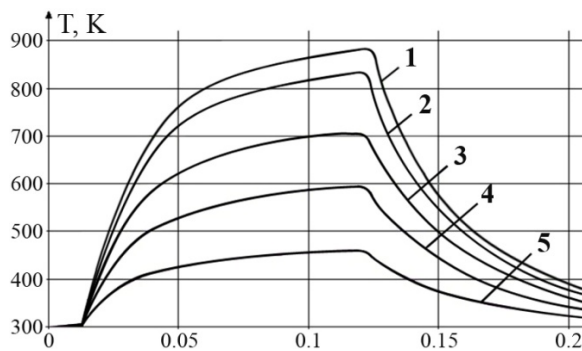


Figure 5. Temperature versus time for the measuring cycle for various coordinates X from the center of the silicon oxide membrane: 1 - 0; 2 - 100 μm ; 3 - 200 μm ; 4 - 300 μm ; 5 - 400 μm .

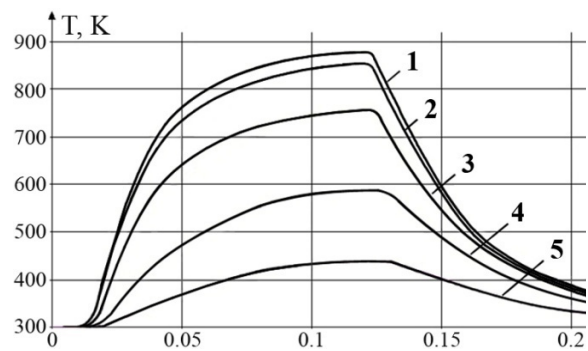


Figure 6. Temperature versus time for the measuring cycle for various coordinates Y from the center of the silicon oxide membrane: 1 - 0; 2 - 100 μm ; 3 - 200 μm ; 4 - 300 μm ; 5 - 400 μm .

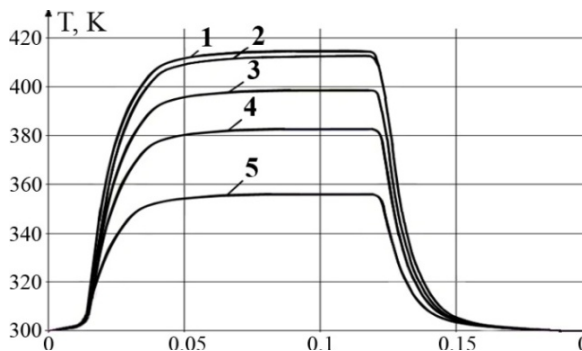


Figure 7. Temperature versus time for the measuring cycle for various coordinates X from the center of the silicon nitride membrane: 1 - 0; 2 - 100 μm ; 3 - 200 μm ; 4 - 300 μm ; 5 - 400 μm .

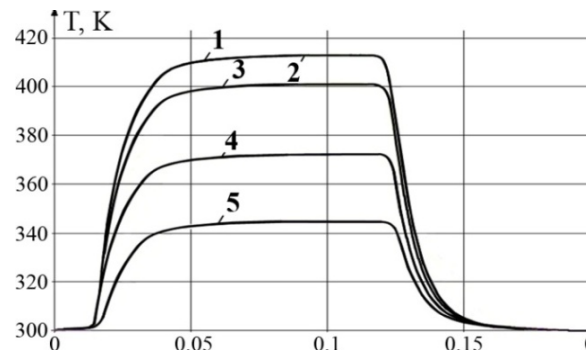


Figure 8. Temperature versus time of the measuring cycle for various coordinates Y from the center of the silicon nitride membrane: 1 - 0; 2 - 100 μm ; 3 - 200 μm ; 4 - 300 μm ; 5 - 400 μm .

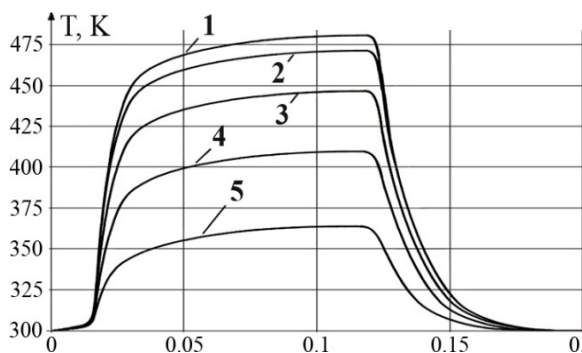


Figure 9. Temperature versus time for the measuring cycle for various coordinates X from the center of the four-layer membrane: 1 - 0; 2 - 100 μm ; 3 - 200 μm ; 4 - 300 μm ; 5 - 400 μm .

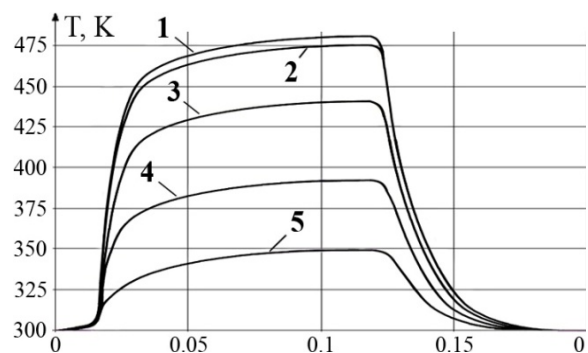


Figure 10. Temperature versus time for the measuring cycle for various coordinates Y from the center of the four-layer membrane: 1 - 0; 2 - 100 μm ; 3 - 200 μm ; 4 - 300 μm ; 5 - 400 μm .

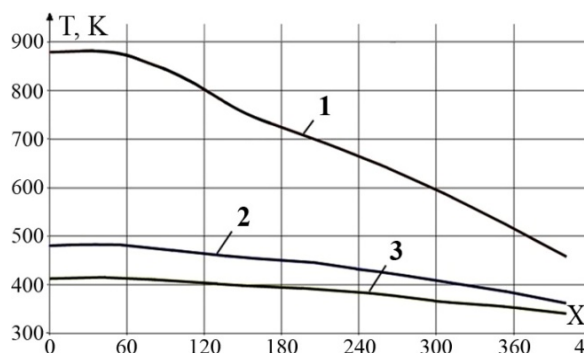


Figure 11. Temperature versus heat for coordinates X at the moment of the highest heat of the sensitive layer area: 1 - silicon oxide membrane; 2 - four-layer membrane; 3 - silicon nitride membrane.

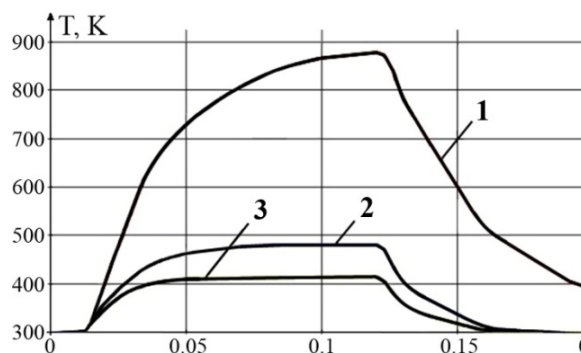


Figure 12. Temperature versus time of the measuring cycle in the center of the membrane: 1 - silicon oxide membrane; 2 - four-layer membrane; 3 - silicon nitride membrane.

3. Results and discussion

Temperature distributions for membranes of different dielectric materials in the measuring mode of a semiconductor gas sensor were obtained. The character of these distributions is uniform and similar for various membranes. This indicates the suitability of the simulated configuration of resistive heaters for semiconductor gas sensors.

Maximum temperature on all dielectric membranes was reached on the plot of 100 - 120 ms from the start of the measuring cycle. For the silicon oxide membrane, the maximal temperature was about 610 oC, for the silicon nitride membrane, it was about 140 oC and for the silicon oxynitride membrane (four-layer membrane) it was about 210 oC. It visually demonstrates the best heat-insulating properties of the silicon oxide membranes.

The simulated membrane structure with the area of the silicon oxide membrane equals 1 mm² and the heating region area of the resistive heater about 0.3 mm² provides the required heat-insulating properties to measure the concentration of a large number of gases. Further decreasing of the heating region area, in accordance with the simulated, surely, will make heat-insulating properties of this membrane structure suitable for use as the basis of sensitive elements for semiconductor sensors of any gases.

On the other hand, the simulation of temperature distribution on the silicon nitride membrane structure has demonstrated the significant heat dissipation through the substrate during the measuring cycle. It significantly decreases the temperature of the sensitive layer area and does not allow obtaining the required conditions for measurement of the concentration of most gases. Therefore, the usage of the silicon nitride membrane structure as the basis for sensitive elements for semiconductor gas sensors is advisable only in the case of improving its heat-insulating properties. For this purpose, it is necessary to reduce the heating region area of the resistive heater or, with the presence of technological opportunities, to increase the area of the membrane. At that, both of these solutions will significantly complicate the process of the production of sensitive elements. Thus, the selection of a silicon nitride film as the heat-insulating membrane material of sensitive elements for semiconductor gas sensors cannot be considered as optimal.

Along with the heat-insulating properties, not less important a selection criterion for the membrane material is the accuracy of achieving the temperature at measurement of the gas concentration and its stability during the measuring period.

As can be seen from the obtained and presented dependencies, silicon nitride membrane can be characterized by a lesser time to achieve and better stability of gas concentration measurement temperature, than can silicon oxide membrane. In the simulation, the silicon nitride membrane was

characterized by a relatively short period of heating during the temperature measuring process, about 40 ms, and a long period of relative temperature stability for measurement, about 80 ms. The obtained dependencies for the silicon oxide membrane differ by the absence of temperature stability period in gas concentration measurement. Throughout the entire period of the pulse application, there was observed a significant increase in temperature. This would adversely impact on the selectivity of gas sensors. As such was the case, silicon nitride was more preferable as the membrane material for sensitive elements of semiconductor gas sensors than was silicon oxide.

This material allows the measurement temperature of gas concentration to be stabilized, however, it reduces heat-insulating properties of the membranes to a greater degree than silicon oxide.

Simulated dependencies of temperature versus time in the center of the membranes, made from different dielectric materials, show the greatest suitability of silicon oxynitride as the membrane material. With the same parameters of the pulse on the silicon oxynitride membrane, there was achieved a larger temperature of the sensitive layer area than on the silicon nitride membrane. In addition, during the heating, the silicon oxynitride membrane was characterized by the presence of a temperature stability period for gas concentration measurement with almost the same duration as would be for a silicon nitride membrane. The results of the simulation allow the following conclusions about nitrogen and oxygen contents in dielectric membrane films for sensitive elements of semiconductor gas sensors to be made:

- the increase of oxygen content in membrane film composition improves the heat-insulating properties of the membrane, which contributes to the improvement of gas sensor selectivity;
- the increase of nitrogen content in membrane film composition lengthens the duration of the temperature stability period for the measurement of the gas concentration, which contributes to the improvement of gas sensor sensitivity.

The optimal element composition of dielectric membrane films for sensitive elements of different semiconductor gas sensors should be selected individually, in accordance with the following. The membrane film should contain the minimum amount of oxygen, yet which is sufficient to guarantee the achievement of the required temperature of the sensitive layer during the measurement. Conjointly, in order to increase the period of temperature stability for measurement and improve the accuracy of achieving the required temperature, membrane film should contain the maximum possible amount of nitrogen. Moreover, that the amount of silicon in membrane film also has significant influence on heat-insulating properties of the membrane, time of achieving the measurement temperature of gas concentration and temperature stability during the measurement should be taken into account.

4. Conclusion

The simulation of the temperature distribution on membrane structures with membranes of different dielectric materials with the application to the resistive heater of a rectangular pulse with voltage equal to 1 V and duration equal to 100 ms was carried out, and the results were visualized and presented. In various moments of the measuring cycle of the semiconductor gas sensors were obtained two-dimensional temperature distributions on silicon oxide, silicon nitride and silicon oxynitride (four-layer membrane) membrane structures. Dependencies of temperature versus time for variety coordinates on membranes, temperature versus coordinates at the moment of the highest heating of the sensitive layer area and temperature versus time in the center of membranes are presented. The simulation results were obtained using the software package Synopsys TCAD. On the basis of obtained results were made recommendations in the selection of membrane film material for heat-insulating membrane structures of sensitive elements for semiconductor gas sensors.

The usage of pure silicon oxide or pure silicon nitride as the membrane film material of heat-insulating membrane structures for sensitive elements of semiconductor gas sensors is inexpedient. Silicon oxynitride is more suitable as membrane film material for such membrane structures. Moreover, it is expedient to individually find the optimal element ratio of membrane film for each semiconductor gas sensor depending on its destination. For example, if it is necessary to ensure the high temperature of gas concentration measurement, in the composition of the membrane film oxygen content should prevail over nitrogen content. If it is necessary to ensure the high accuracy of achieving relatively low

temperature of gas concentration measurement, in the composition of membrane film, nitrogen content should prevail over oxygen content. Therefore, it is important to experimentally find the optimal element ratio of membrane film material for the sensitive elements of semiconductor gas sensors for various purposes.

Obtained and presented simulation results and made recommendations allow to reduce the field of required experimental study of heat-insulating materials at dielectric membrane structures development. This simplifies the selection of optimal membrane film composition for dielectric membrane structures of sensitive elements for semiconductor gas sensors.

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