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Development of a 3D-integrated Thermocatalytic Sensor for Combustible Gas Detection

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Summary:
A process to integrate a thermocatalytic sensor on top of a CMOS circuitry is presented. Therefore, COMSOL Multiphysics® simulations are performed to evaluate a heater with an optimized temperature uniformity and a suspended design of the sensor element to achieve thermal decoupling from the substrate. The steps for fabrication are shortly described using ALD materials and a sacrificial layer. An example for a released heater structure is shown.

Keywords: thermocatalytic sensor, 3D-integration, ALD, post-CMOS, pellistor

Introduction

Pellistors are thermocatalytic sensors that are used to detect combustible gases. A realization of a pellistor as a MEMS sensor has already been achieved (micro pellistor) [1]. This reduces the size of the sensor element, decreases the power consumption and increases the mechanical stability compared to the classic pellistor [2]. When mounting the micro pellistors on silicon substrate they have to be manufactured on membranes for thermal decoupling. If a readout circuit for the sensor is to be manufactured, it must either be processed separately or the chip area spared for the sensor in the case of monolithic integration causes high costs.

In order to save chip area and still achieve a monolithic assembly of readout circuit and sensor, the Fraunhofer IMS developed a concept to create free-standing electrically contacted structures by means of a sacrificial layer process combined with ALD deposition, which can be operated on top of a CMOS circuit [3]. Therefore, the concept of pellistors is to be adopted and further developed into a 3D integrated thermocatalytic sensor, which is applied on top of the readout circuit.

Design of the Sensor

The sensors produced by ALD materials are based on the components of a classic pellistor: a heater, an insulating material around the heater and a catalyst layer on the isolating material. Since the structures are smaller than those of micro pellistors, it is necessary to ensure that the heater is dimensioned reasonably to achieve the most homogeneous temperature profile possible. Therefore, simulations with COMSOL Multiphysics® using the “Joule Heating” interface were performed.

Based on [4] a square shaped heater shows the highest temperature uniformity compared to other heater shapes. Instead of fabricating the heater structure directly on pillars resulting in a non-negligible substrate heating along the pillars, a design is chosen where a suspension via legs provides a thermal decoupling to the substrate, as the main temperature drop occurs over the legs. According to the simulations, at a maximum temperature of the heater of 513°C, the temperature drop at the heater itself is only 26°C, while the maximum temperature at the substrate directly below the pillars is 34°C.

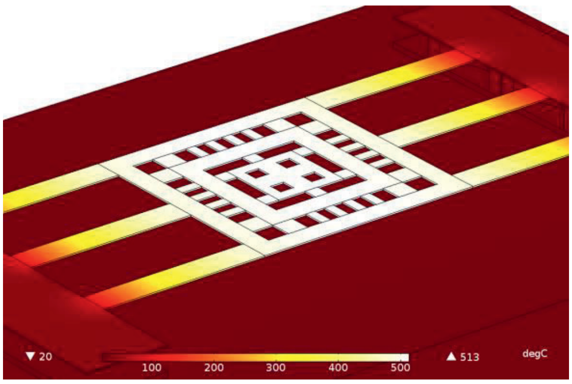

Fig. 1. Simulations with square shaped heater suspended by legs for main temperature drop. Height of pillars defines the distance between the free-standing sensor and the substrate.

Ruthenium as Heater and Catalytic Material

Ruthenium is used as both the catalytic layer and the heater material. Like platinum, ruthenium is a transition metal and shows catalytic activity towards combustible gases. According to [5] ruthenium is even better suited as a catalyst chosen for a pellistor (examined on the basis of CO). Although the material is liable to form a thin oxide layer especially at higher temperatures the catalytic activity still remains.

As the heater is also used to measure the temperature change caused by reaction at the catalysts surface a high and linear temperature coefficient is beneficial for a reliable measurement. According to tests the sheet resistance of ruthenium is nearly linear up to 400°C. This gives a temperature coefficient of approximately $2 \cdot 10^{-3}\,K^{-1}$ (in comparison $3{,}92 \cdot 10^{-3}\,K^{-1}$ for platinum) which makes ruthenium suitable for temperature measurement.

Fabrication of the Sensor

To fabricate a thermocatalytic sensor as a free-standing element, a sacrificial layer to set the distance between sensor and substrate with the circuitry has to be deposited first. After that holes or trenches are etched with a stop at the contact pads for electrical supply. The highly conformal deposition of an ALD layer provides the sensor with its heater material which can be structured. The sacrificial layer can then be etched so that the sensor structure is released. A released structure of a square shaped heater can be seen in Fig. 2.

To trransform the sensor element to a pellistor like structure an Al_2O_3 layer can be deposited before etching the trenches into the sacrificial layer and another Al_2O_3 layer above the heater material encapsulates the heater. Eventually, a catalyst layer on top of the upper Al_2O_3 layer must be deposited.

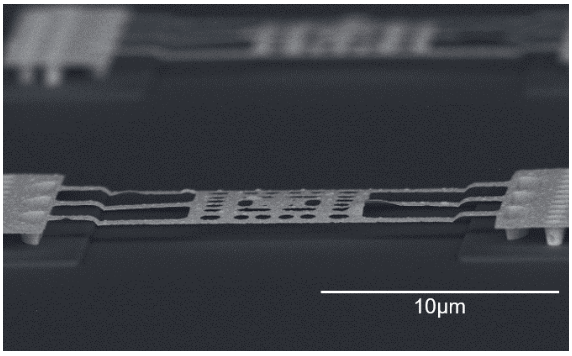

Fig. 2. SEM image of a released ruthenium square shaped heater with a distance of 1 µm to the substrate.

Conclusion and Outlook

A possibility to fabricate a free-standing gas sensor in a post-CMOS process was introduced. Therefore, an optimized square shaped structure was presented to achieve a high temperature uniformity and a design of a heater held by suspension legs was shown as a way to realize a thermal decoupling from the substrate without etching a membrane. Process flows to fabricate an unencapsulated heater as a thermocatalytic sensor and an encapsulated pellistor like element were described and actual structures were shown.

In future work the fabricated structures will be measured and characterized in terms of its properties. The encapsulated versions of the sensor will be completed and characterized as well.

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