µHeater on a Buckled Cantilever Plate for Gas Sensor Applications

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Abstract: Electro-thermal simulation and analysis of a micro-heater (µHeater) on a buckled cantilever structure for gas sensor applications is reported. The buckled cantilever allows the sensor plate to be suspended for thermal insulation. Both Structural Mechanical Simulation and the Joule Heat Transfer Simulation were integrated using the Finite Element Analysis package COMSOL 4.2a. The main objective of our work is to calculate the appropriate parameters needed to generate 350 ºC on the plate surface, which is the working temperature targeted for our gas sensor platform. The analysis results suggest that the working voltage for the µHeater should be around 0.2 V. More work is being done to calculate the power consumption with the simulation results. The simulation will also allow us to verify the efficiency of the current design and will suggest if any modification is needed.

Keywords: MEMS, micro-heater, micro-hotplate, gas sensor, buckled cantilever.

1. Introduction

In semiconductor gas sensors, the base of the gas detection is the interaction of the gaseous species at the surface of the semiconducting sensitive material. This interaction is possible at elevated temperatures and allows charge transfer to take place between the absorbed species and the sensitive material. The change of the concentration of the free charge carriers is translated into a change of the overall resistance of the sensing layer. The most widely used materials for this purpose are metal oxides like SnO_2. But, a single metal-oxide material can sense many gases, implying that selectivity is a major concern. Selectivity can be improved by varying the operating temperature of the sensor. Since the chemical reactions at the surface of the sensor material are functions of temperature, sensitivity strongly depends on the sensor's operating temperature. This is why a heat generator transducer or micro-hotplate is so important for this application.

Micro-hotplates also allow the reduction of the sensor's power consumption. Other authors have reported the design, simulation and/or fabrication of µHeaters for low power applications [1-4] and there is a growing interest in the use of polymeric substrates and structures for such devices, due to their flexibility, low cost and fabrication simplicity [4-6].

We have chosen the Buckled Cantilever design [11-13] as a compliant out-of-plane structure for our transducer. Taking advantage of the out-of-plane characteristic, our active device is mounted on a plate between two cantilevers for thermal insulation once the structure is assembled; we call this structure "Buckled Cantilever Plate" (BCP). It is worth to mention that the µHeater is electrically routed to the contact pads located at the anchors, through the buckled cantilever length.

Devices have already been fabricated; see Figure 1, using silicon as the substrate and non-photosensitive polyimide PI2611 as the structural layer for the BCP structures. Characterization of such devices is ongoing. In this paper, we report the simulation of the fabricated micro-hotplates design mounted on a BCP structure. The important characteristics of the design and fabrication will be discussed in the following section.

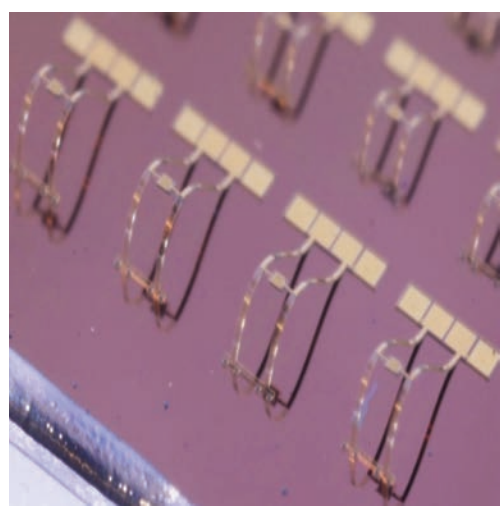

Figure 1 Fabricated, released and assembled BCP gas sensor devices.

2. Design and Fabrication

The layout for our micro-hotplate is shown in Figure 2. As shown, the heater element consists of a metal layer patterned in double-spiral fashion. The width of the spiral lines is 5um and separation between them is 10um. An additional polyimide and metal layer are needed to create a complete gas sensor, but for simulation purposes they are not included. The buckled cantilever structure is simply two cantilevers parallel to each other with the sensor plate attached between them.

The starting material for our fabrication process is a 4-inch silicon wafer with a 300nm SiO_2 layer. A 2µm α-Si layer is deposited as sacrificial layer for the freestanding features. After that, typical photolithography and dry etch with SF6 are used to pattern dimples and anchors. The polyimide PI2611 is then spun and cured to 5um, followed by the metal lines deposition. Different metals are used for the uHeater: Titanium/Gold bilayer for the connection lines and Tungsten, which has a slightly higher temperature coefficient of resistance, is used as the heating material. Both layers are patterned using lift-off technique. To fabricate a complete gas sensor, a second layer of polyimide is spun and cured followed by Titanium/Gold lift-off to pattern the electrodes. After this, both polyimide layers are patterned by dry etch. Finally, the devices are released using a XeF_2 dry etch. The fabrication process is detailed in Figure 3.

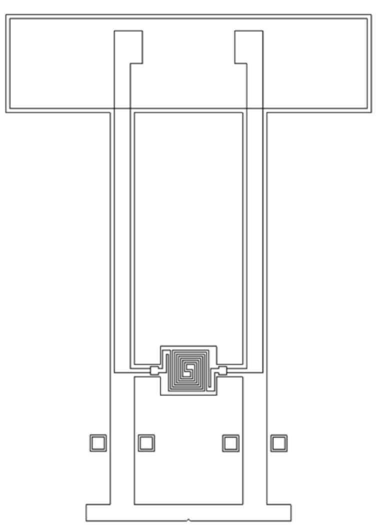

Figure 2 Top View of BCP gas sensor Layout.

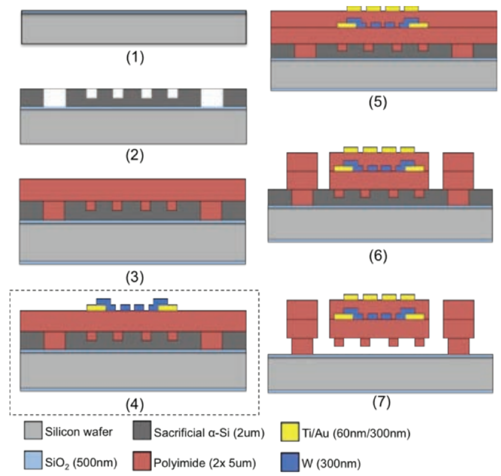

Figure 3 BCP gas sensor fabrication process. The highlighted step (4) shows a finished hotplate without the electrodes, as it was simulated for this paper.

3. Electro-Thermal model

Joule heating effect, also called resistive heating, explains the behavior of our µHeater. The electric current through the double spiral generates heat Q, which is proportional to the square of the magnitude of the current density J. The electrical resistivity ρ is the coefficient of proportionality (eq. 1).

$$Q = \rho |J|^2 \qquad (1)$$

In order to get a fully coupled equation to express the electric potential V as the solution variable (eq. 2), some other relations have to be taken into account:

a) Electrical resistivity is the reciprocal of the temperature dependent electrical conductivity σ.
b) Current density J is proportional to the electric field E.
c) Electric field E equals the negative of the gradient of the potential V.

$$Q = \frac{1}{\sigma}|J|^2 = \frac{1}{\sigma}|\sigma E|^2 = \sigma|\nabla V|^2 \qquad (2)$$

As mentioned before, the electrical conductivity is also temperature dependent. Eq. 3 defines the electrical conductivity as function of temperature T.

$$\sigma = \frac{1}{\rho_0(1+\alpha(T-T_0))} \qquad (3)$$

Where:

σ_0: conductivity at reference temperature.
T_0: reference temperature.
α: temperature coefficient of resistivity.

4. Simulation Setup

The purpose of our simulation is to investigate the working voltage of our μHeater design, as well as the behavior of the BCP structure in its assembled position while the μHeater is active. For this reason we are using the multiphysics capabilities of COMSOL to integrate the mechanical and the electro-thermal simulations. The simulation is divided in two different studies. In first instance we have simulated the mechanical assembly of a BCP structure using the Solid Mechanics module for the first study, followed by the integration of the Joule Heating module for the simulation of the μHeater metal layer in the second study.

4.1 Study 1: BCP assembly simulation

The BCP assembly is achieved by applying a displacement or a force to its free ending edge. For our particular case we have parametrically evaluated small displacement to the bottom free end edge of the BCP structure. The displacements have been set so that the edge moves from its initial position to its assembly position (~216μm) in the "y" direction (**Fig. 4**), in steps of 1μm for each solution. For the boundary conditions of the Finite Element Analisys (FEA), we have set the bottom edges of the anchor features as fixed constraints, so they maintain direct contact with the substrate, while the free end bottom edge of the BCP structure has a constrain in the Z-axis at -2μm so it can move freely in the XY plane. The last consideration represents a virtual plane simulating the substrate's top surface. In this way the cantilever edge will slide in described displacement and will not be able to go beyond this virtual surface in the "Z" direction creating non-realizable solutions to our problem. Once the assembly is simulated the results can be saved so they can be used by the second study.

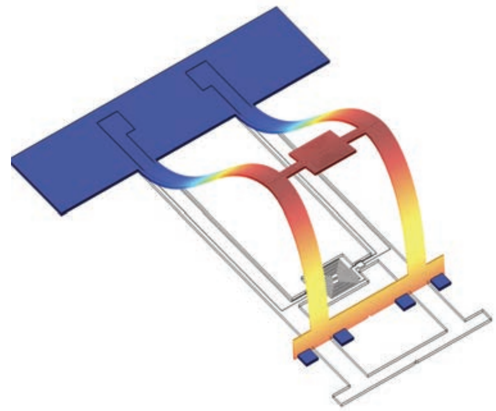

Figure 4 Assembled BCP with parallel plate to the substrate.

4.2 Study 2: μHeater simulation

Once the BCP study is performed, we can use any of the saved results to perform the second study. This means that the second study solution (heat generation) can be evaluated in each deformation step of the BCP structure.

To execute the second study we specify the corresponding boundary conditions to the metal layers. It is expected that by inducing a current to the circuit heat will be generated in the tungsten coil, due to its physical properties. Initially we define a face of one of the contact pads as the ground terminal and a face of the other contact pad defined with an electrical potential. By performing a parametric value for the electrical potential we can discover the required voltage to generate approximately 350Cº, which is the working temperature for a potential gas sensor. The parametric potential value was set to go from 0.2V to 0.215V. Because we are dealing with temperature, we need to set boundary conditions for this physic too. The initial temperature of the system is set to room temperature (293.15 Kelvin). Finally, by setting the top surfaces of the entire structure as boundaries for convective cooling the model is ready to be solved by the second study for the Joule Heating problem.

5. Results

After coupling both studies we were able to display the results in 3D graphs. The mechanical simulation gives the opportunity to show the deformation of the structures lifting the μHeater to a height of 258μm, see **Fig. 4**. The selected working temperature for the gas sensor was achieved by applying 0.212V, getting a simulated temperature of 351.48ºC (**Fig. 5**). In **Fig. 6** the assembled BCP with the working heater is shown. We can see that the heat distribution is pretty even and concentrated only in the μHeater, with the temperature ranging from approximately 300ºC to 351ºC.

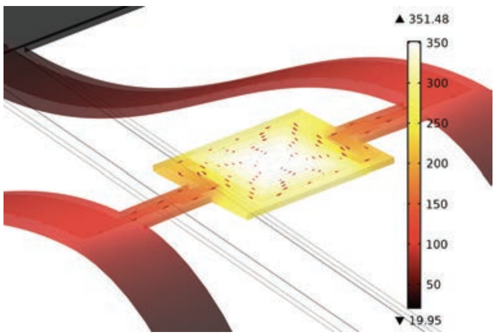

Figure 5 Heat flux in the μHeater. Working Temperature 351.48ºC using 0.212Volts.

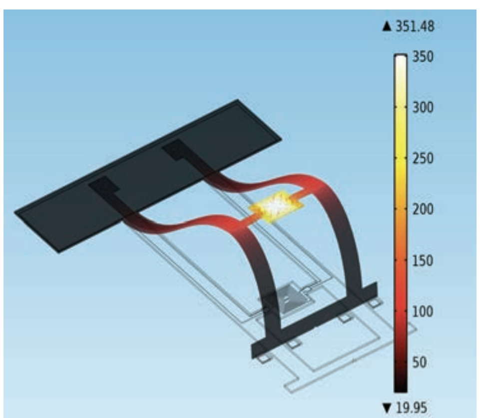

Figure 6 Assembled BCP and μHeater coupled simulations.

6. Conclusions & Future Work

In this work we have demonstrated the use of COMSOL Multiphysics by coupling the Structure Mechanics and Joule Heating modules. The needed voltage to generate the required temperature for our gas sensor was found to be approximately 0.212V. The devices have been fabricated and are currently being characterized. A variation of the dimensions parameters of the BCP as well as the vertical plate configuration has been fabricated (**Fig. 7)**. Further work includes the comparison between the simulated results and the experimental data. The μHeater simulation has provided us with good insight on our device's operation and has not revealed any significant issues in need of alteration on the BCP structure.

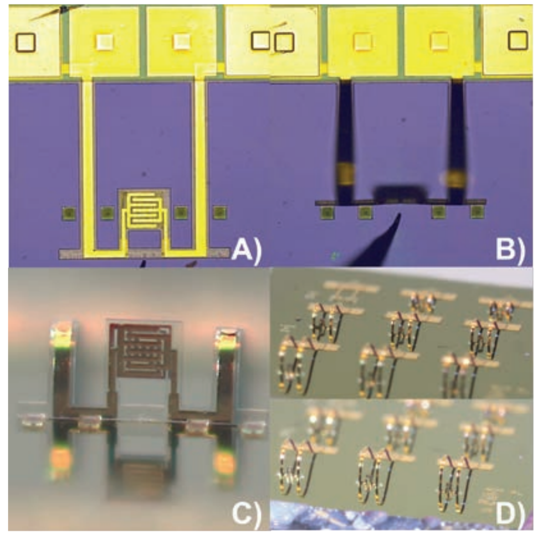

Figure 7 A) Top view of fabricated and released Polymer Gas Sensor on a BCP. B) Top View of assembled Polymer Gas Sensor BCP. C) Front View of vertical assembled Polymer Gas sensor BCP. D) Chip with assembled Polymer Gas Sensor BCPs.

7. References

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