Design and simulation of resistive SOI CMOS micro-heaters for high temperature gas sensors

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Abstract. This paper describes the design of doped single crystal silicon (SCS) micro-hotplates for gas sensors. Resistive heaters are formed by an *n*+/*p*+ implantation into a Silicon-On-Insulator (SOI) wafer with a post-CMOS deep reactive ion etch to remove the silicon substrate. Hence they are fully compatible with CMOS technologies and allows for the integration of associated drive/detection circuitry. 2D electro-thermal models have been constructed and the results of numerical simulations using FEMLAB® are given. Simulations show these micro-hotplates can operate at temperatures of 500°C with a drive voltage of only 5 V and a power consumption of less than 100 mW.

1. Introduction

The market for portable, handheld gas monitors is still relatively small in spite of an increasing demand from within the environmental, automotive and medical industries. The relatively high power consumption of present commercial gas sensors makes them impractical for battery powered applications. For example, commercially available pellistors need the catalyst to be heated up to around 500°C and have a typical power consumption of 350 to 850 mW [1]. Taguchi type resistive gas sensors, the most commonly used gas sensor, requires around 800 mW for an operating temperature of between 300 and 400°C [2]. Another problem associated with these sensors is the semi-manual manner in which they are fabricated, thus making them expensive to make in high volume compared to microelectronic chips. Developments over the last 10 years in silicon microtechnology have made it possible to fabricate low power, low cost and small micro-hotplates that can be used for gas sensors [3-7]. However, commercial exploitation of these micro-hotplates has not yet been fully realised. Platinum based micro-hotplates are most widely investigated [3, 4], since platinum is a thermally stable material and the reliability of this type of resistive micro-hotplate is excellent. However, platinum is not a CMOS compatible material and as such micro-hotplates cannot be fully integrated with drive/detection circuitry. Thus the fabrication process is still relatively expensive. Polysilicon and aluminium based micro-hotplates have also been fabricated and characterised [5, 6]. Although they are CMOS compatible, they suffer from poor long term stability due to the grain boundary of polysilicon being highly reactive and aluminium suffering from electro-migration especially at high temperatures. Udrea *et al*. [7] have recently reported the use of SOI-CMOS based MOSFETs as micro-hotplates. This type of micro-hotplate provides simple temperature control via the applied gate voltage and has better thermal stability and durability than polysilicon as the heater is made of single crystal silicon (i.e. the MOSFET channel). However its operating temperature is limited to less than 400°C in SOI CMOS technology, because of the bipolar turn-on and the use of aluminium interconnects.

In this paper, novel SOI based micro-hotplates employing doped SCS as the heater material are proposed and their thermal characteristics simulated. These micro-hotplates can be operated at higher temperatures than MOSFETs (e.g. 300-600°C) with lower power consumption, but still with the possibility of integrating circuitry.

2. SOI micro-hotplate structures

One issue in using silicon as a resistive heater material is that its resistivity is much higher than that of metals (the resistivity of *n*-silicon of 10^{19} cm^{-3} doping is 6×10^{-5} Ωm [8] and pure aluminium is 2.65×10^{-8} Ωm [2]). However the thermal conductivity is almost the same as metals (thermal conductivity of silicon is 168 W/m/K and aluminium is 236 W/m/K [2]). The power P of a resistive heater is given by

$$P = R_H I^2 + R_T I^2 \qquad (1)$$

where R_H and R_T are resistances of the heater and track, and I is electric current. The first term is the Joule heat generated to raise the temperature of membrane. On the other hand, most of the heat generated by the tracks is dissipated to the substrate. Moreover, a high track resistance will be an issue as it will reduce the voltage dropped across the heater. Therefore, wider tracks, which have lower resistance, are preferred. However, from a thermal point of view, wider tracks cause more heat to be dissipated along the tracks to the substrate. To solve these conflicting design issues, two structures are proposed: sector shape silicon tracks and tungsten tracks.

A cross-section of an SOI calorimeter employing this micro-hotplate is shown in figure 1 and the micro-hotplate design with sector shape silicon tracks is shown in figure 2(a). The micro-hotplate comprises a silicon nitride/silicon dioxide membrane of radius 282 μm in which a silicon resistive heater of radius 75 μm is sandwiched. This structure may be fabricated through a standard SOI CMOS process. Apart from the area used as heater and tracks, the whole active silicon layer is back etched to decrease the thermal losses of the membrane. The buried oxide layer acts as an etch stop and thermally isolates the sensing area, further reducing power loss. Silicon is doped simultaneously with the source and drain regions since they have the highest concentration in MOS devices and resulting in minimum resistance of the tracks. The silicon substrate can be etched away by a deep reactive ion etch (DRIE) process to produce near vertical walls and hence minimise the chip size. The advantage of this silicon track design compared with a straight one, of constant width, is that it generates more heat in the inner region of the track and so can be used more efficiently to raise the temperature of heater area. The silicon track is connected to metal outside the membrane, where the temperature approximately equals that of ambient. This design does not contain any metals in the heater region, thus can be operated at significantly higher temperatures (in excess of 300 ^{o}C). The shapes of both membrane and heater have been chosen to be circular so to reduce the possibility of fracture due to stress. The width of the resistive heater rings has been varied with the outer ring being wider. This has been implemented as the outer region loses more heat through conduction to the membrane than the inner region, thus the structure will improve the temperature uniformity. In addition, there is a silicon heat spreading plate at the central region of micro-hotplate to again enhance temperature uniformity.

The design of micro-hotplates with tungsten tracks are shown in figures 2(b) & 2(c) and a cross-section of a resistive gas sensor employing tungsten track micro-hotplate are shown in figure 3. Tungsten is chosen as a material to reduce the track resistance and to reduce the effect of electro-migration, and because it is used in high-temperature applications. The shape shown in figure 2(b), which is referred to as 'tungsten track, large resistance' has a nominal resistance of 760 Ω. The design in figure 2(c) is referred to as 'tungsten track, small resistance', has a lower resistance of *ca* 240 Ω and hence lower operating voltage. In this process, the second metal layer can be used as a heat spreading plate and the third metal layer can be used as resistive electrodes. Both the silicon track structure and the tungsten track structure can be integrated with electronic circuitry as shown in figure 3.

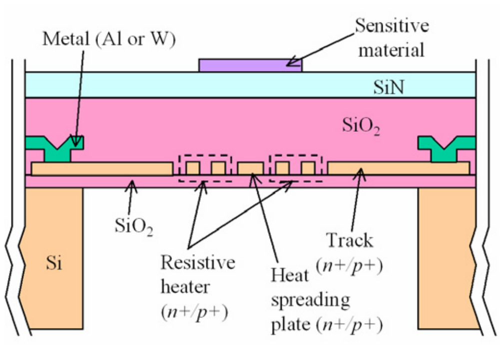

Figure 1. Structure of a calorimetric gas sensor employing SCS micro-hotplates with silicon track.

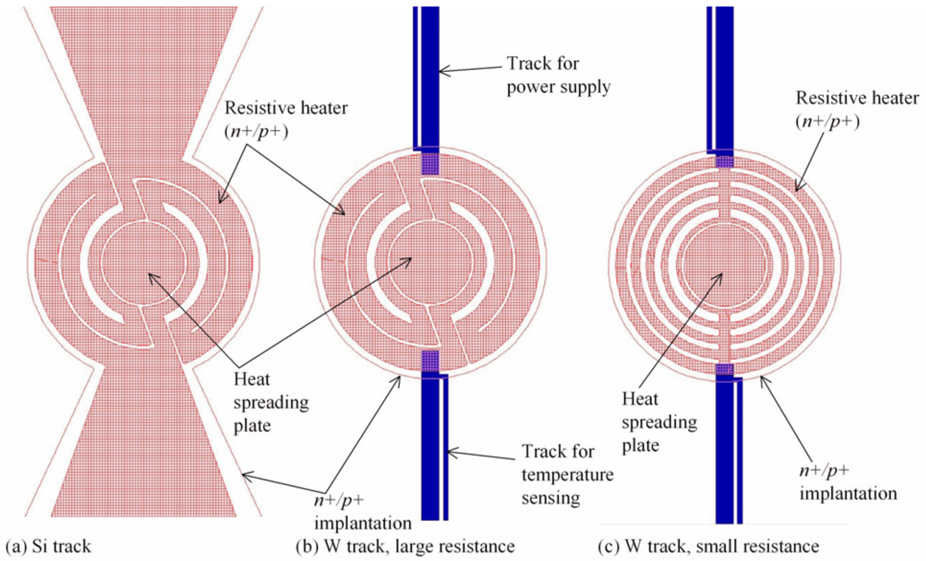

Figure 2. Design of micro-hotplates employing SCS resistive heaters.

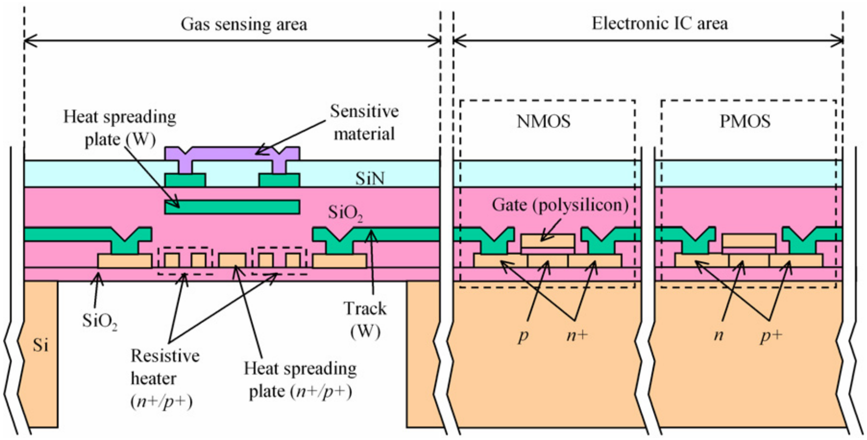

Figure 3. Structure of a resistive gas sensor employing SCS micro-hotplates with tungsten track. The gas sensor is integrated with MOSFETs.

3. 2-D electro-thermal modelling of micro-hotplates

In order to carry out 2-D electro-thermal simulations, it is necessary to create a finite element model of these micro-hotplates. The Joule heating and heat dissipation are described in the following equations:

$$\sigma(T)(\nabla V)^2 = P_{conduction} + P_{convection} + P_{radiation} \quad (2)$$

$$\nabla \cdot [\sigma(T)\nabla V] = 0 \quad (3)$$

$$\sigma(T) = 1 \Big/ \left\{ \rho_a \left[1 + \alpha_1 (T - T_a) + \alpha_2 (T - T_a)^2 \right] \right\} \quad (4)$$

where $\sigma(T)$ is electrical conductivity, T is temperature, T_a is the ambient temperature (27°C), V is electric potential, ρ_a is resistivity, α_1, α_2 are temperature coefficients of resistance, $P_{conduction}$, $P_{convection}$, $P_{radiation}$ are power losses per unit volume caused by each mechanism. The mechanism of power loss through the membrane is denoted as:

$$P_{conduction} = -\nabla \cdot (\kappa \nabla T) \quad (5)$$

where κ is thermal conductivity and calculated as follows:

$$\kappa = (t_{SiN}\kappa_{SiN} + t_{SiO2}\kappa_{SiO2} + t_{Si}\kappa_{Si} + t_w\kappa_w)/(t_{SiN} + t_{SiO2} + t_{Si} + t_w) \times c \quad (6)$$

where t is the thickness of each film and c is the correction factor to consider the different thickness of membrane denoted as

$$c = (t_{SiN} + t_{SiO2} + t_{Si} + t_w)/(t_{SiN} + t_{SiO2}). \quad (7)$$

The following values are assumed for the thermal conductivity of each material: κ_{SiN}=20 W/m/K, κ_{SiO2}= 1.4 W/m/K, κ_{Si}= 168 W/m/K, and κ_W=177 W/m/K. For convection, i.e. power loss to the ambient air, is modelled by [4]:

$$P_{convection} = \left\{ \left[0.104(T - T_a) + 4.129 \times 10^{-4} (T - T_a)^2 \right] \Big/ 5.0 \times 10^{-7} \right\} \Big/ (t_{SiN} + t_{SiO2}) \quad [mW/m^3] \quad (8)$$

The denominator, which is the thickness of membrane, in equation (8) is used to obtain the value per volume. Radiation power loss is described as follows:

$$P_{radiation} = 2\varepsilon\sigma(T^4 - T_a^4)/(t_{SiN} + t_{SiO2}) \quad (9)$$

where the emissivity ε is assumed to be unity and the value of the Stefan-Boltzmann constant σ is 5.67×10^{-8} W/m^2/K^4. The edge of membrane is assumed to be at ambient temperature.

4. Results of simulations and discussion

The commercial software FEMLAB® (COMSOL, Version 2.3.0.153) was used to solve the electro-thermal problem with a mesh of triangles generated automatically. Temperature contours within the membrane at 500°C are shown in figure 4 and the relative contribution of each heat dissipation path is shown in figure 5. From figure 5, it is concluded that conduction is the main power loss mechanism. Power loss through air and radiation are much less than the reported value (e.g. convection heat loss is 2/3 of total in [4]). This is because the area of heater is much less than reported in [4] (0.5 mm^2 compared to 0.018 mm^2). Therefore, the results here will focus on the issue of conduction. Figure 4 shows that temperature profiles of all micro-hotplates are almost uniform without any central hot spots. Despite wide tracks, the silicon track micro-hotplate provides a nearly circular temperature profile. This is the result of balancing the heat generated at the inner region of tracks with the dissipated power through the tracks. As for the tungsten track micro-hotplates, the small resistance design shows an elliptic temperature profile with a higher temperature region around the tracks, whilst the large resistance design shows circular temperature profile. The reason for this is the large amount of Joule heat caused by the large current required to operate the small resistive heater.

Figure 6 shows that power consumption of all of the micro-hotplates to be less than 100 mW when operated at 500°C. This value is ideal for handheld, battery powered applications. The silicon track micro-hotplate consumes about 20 mW more power than the tungsten tracks. This is due to the larger conductive losses and Joule heat generated in silicon tracks and thus it is less efficient. Figure 7 shows that the tungsten spreading plates can significantly improve temperature uniformity. This design reduces the overall temperature variance from ±35°C to only ±15°C.

Figure 8 shows the required voltage of each micro-hotplate. Tungsten track, small resistance micro-hotplates can be operated at the lowest voltage and it is the only micro-hotplate to operate at 500°C for less than 5 V (standard battery voltage).

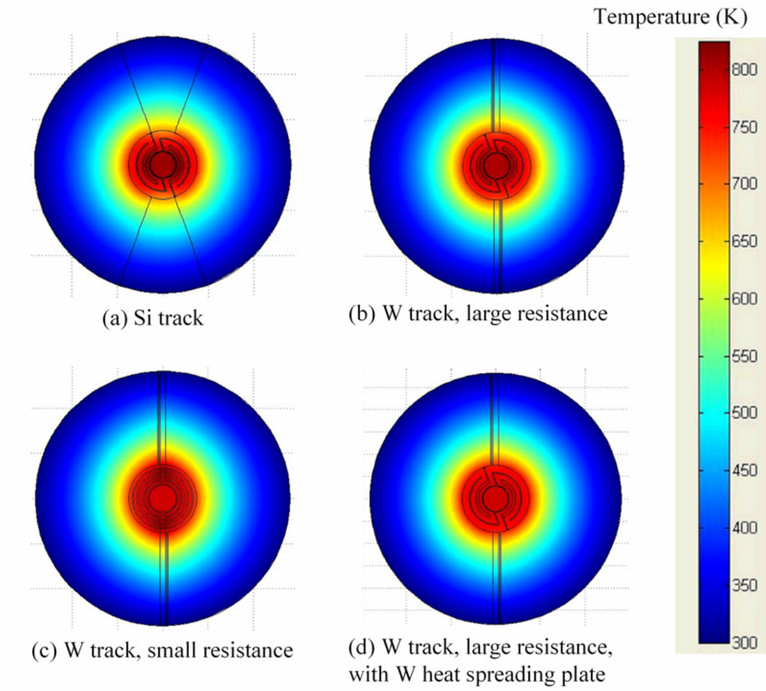

Figure 4. Temperature profiles of SCS resistive micro-hotplates at 500°C.

5. Conclusions and further work

Two types of micro-hotplates, for gas sensors, employing single crystal silicon as resistive heaters are proposed. Both designs are fully compatible with a SOI CMOS process and hence can be integrated with drive and detection circuitry. In addition, they can operate at temperature of 500°C with a power consumption of less than 100 mW. The first design employs sector shaped tracks made of *n*+ or *p*+ doped silicon and is suitable for use in a micro-calorimeter without any metals in the heater area. This design can be fabricated using a standard aluminium SOI CMOS process. The second design comprises of resistive heaters made of *n*+ or *p*+ silicon with tungsten tracks. This concept reduces the resistance of the heater to 240 Ω and can be operated at standard battery voltage of 5 V. Temperature uniformity of this micro-hotplate is further improved by a heat spreading plate with a temperature variance of *ca* ±15°C. These doped single crystal silicon micro-hotplates are presently being fabricated.

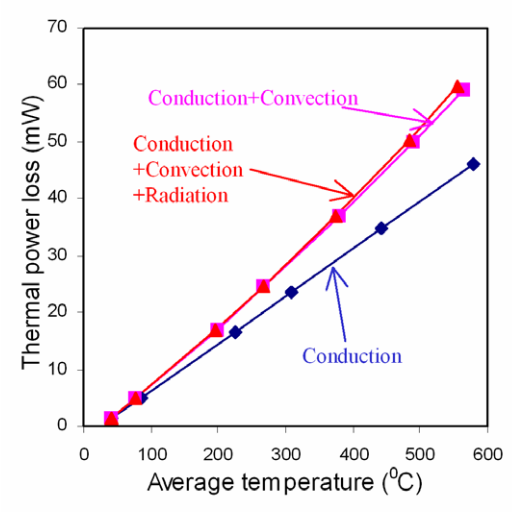

Figure 5. Contribution of each heat dissipation mechanism.

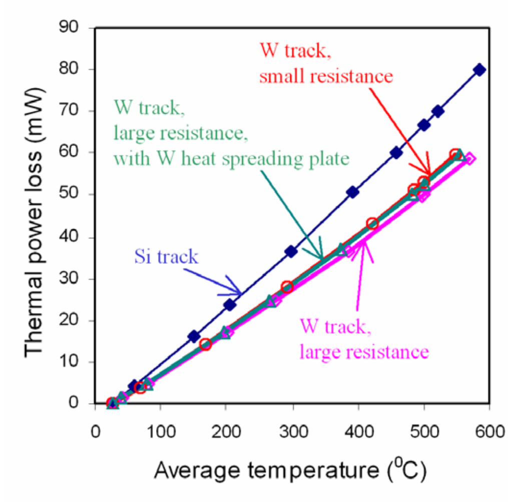

Figure 6. Thermal power loss of each micro-hotplate.

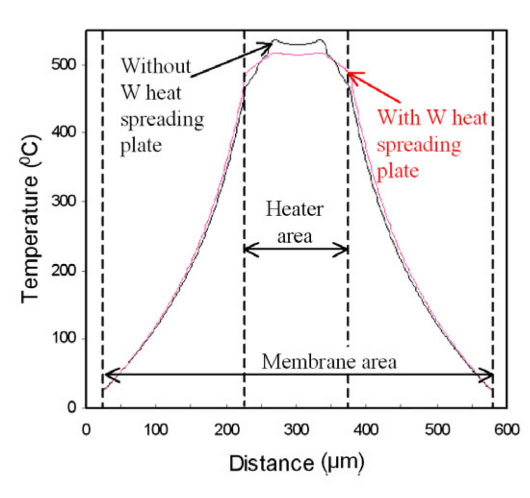

Figure 7. Temperature profiles of tungsten track micro-hotplates.

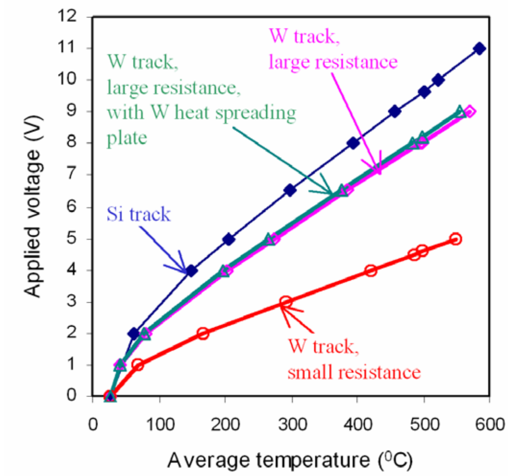

Figure 8. Operating voltage of each micro-hotplate.

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