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Thermal modelling of a porous silicon-based pellistor-type catalytic flammable gas sensor with two supporting beams

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Abstract

A three-dimensional transient thermal mathematical model of a porous silicon based pellistor with two supporting beams was developed. The model was numerically solved using the implicit alternating-direction finite difference method. A computer program written in ANSI C and run on a VAX/VMS computer was utilised to study the influence of the power consumption and the main geometrical dimensions (membrane, beam and heater size) of the pellistor mentioned above on its transient and steady-state thermal behaviour. It was found that considerable improvement in the thermal behaviour of the pellistor could be achieved by reducing the membrane size (length and width). The optimal beam length was determined as 100 μm. By comparing the main sources of energy dissipation it was found that energy was lost predominantly through the heat conduction into the supporting beams. © 2000 Elsevier Science Ltd. All rights reserved.

Keywords: Thermal model; Pellistor; Simulation

1. Introduction

Pellistors are catalytic devices measuring the heat evolved during controlled combustion of flammable gas in the ambient air [1]. The heat evolved during the combustion process can be easily related to the concentration of the flammable gas. To initiate the combustion reaction for most flammable gases, the temperature at the catalytic layer should be maintained at around 400°C. This, however, requires power consumption, which can easily exceed the corresponding limit in transducers. For this reason, the optimal thermal design of micro-pellistors is of primary importance. Pellistors, in which the membrane where the catalytic layer is attached is supported by beams, require less energy to achieve their thermal target compared to those utilising membranes directly attached to the main body of the pellistor [2]. The average temperature at the catalytic layer of the pellistor where the exothermic combustion reaction takes place is influenced mainly by the power consumption and the pellistor geometrical dimensions. Among the geometrical dimensions, the membrane and the beam size are of utmost importance. A cost effective approach in optimising those dimensions is the numerical simulation of the corresponding thermal model of the pellistor. In the current paper, the development of a mathematical model describing the thermal behaviour of a porous silicon based pellistor with two supporting beams is outlined. The optimisation of the pellistor dimensions by numerical simulations is reported.

2. Development of the mathematical model and its numerical solution

The pellistor modelled in the current study is schematically presented in Fig. 1. It consists of two rectangular beams supporting a rectangular membrane of silicon nitride (Si_3N_4). The n-Silicon (n-Si) heater and the porous Si layer, both rectangular in shape, are attached to the membrane. The Pt slabs connecting the n-Si heater to the power supply and the Pt resistor slab are embedded in the Si_3N_4 supporting beams (Fig. 1). To simplify the calculations the width of the membrane was assumed to be identical to that of the beams and both Pt slabs mentioned above were combined in one Pt slab running along the membrane and the beams (Fig. 2). It

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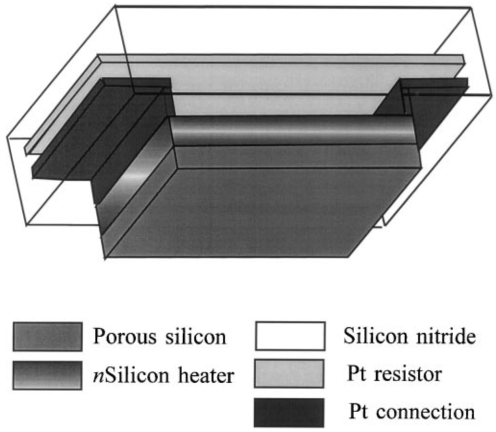

Fig. 1. Scheme of the membrane and the supporting beams.

was assumed that the ends of the beams attached to the main body of the pellistor were at ambient temperature and that the power consumption was located in the heater only (Figs. 1 and 2).

Because of the symmetry of the pellistor (Fig. 1), the mathematical model considers one-fourth of the membrane and half of the corresponding adjacent beam only (Fig. 3).

The following three main sources of heat loss were taken into account: (i) heat radiation; (ii) heat conduction between the beams and the main body of the pellistor; (iii) conduction in ambient air.

The heat conduction within the membrane and the beams of the pellistor and in the air surrounding them is described

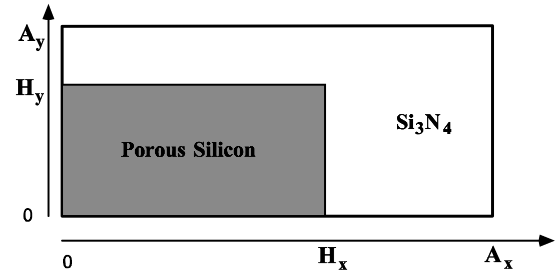

Fig. 3. Scheme of one fourth of the pellistor.

by the three dimensional equation of heat transfer (Eq. (1))

$$\frac{\partial T}{\partial t} = \alpha_i \left(\frac{\partial^2 T}{\partial X^2} + \frac{\partial^2 T}{\partial Y^2} + \frac{\partial^2 T}{\partial Z^2} \right) + S \quad (1)$$

where T is the temperature; X, Y and Z the spatial coordinates; $\alpha_i = k_i/\rho_i C_i$ is the thermal diffusivity of the ith phase (Si, Si_3N_4, Pt or air); k_i is the thermal conductivity; ρ_i and C_i are the density and the heat capacity of the corresponding phase, respectively. The heat source (S) in the heater is described by Eq. (2) while outside the heater $S = 0$

$$S = Q/V_h \rho_s C_s \quad (2)$$

where Q is the heating power, V_h is the volume of the heater ($V_h = (Z_1 - Z_2)H_x H_y$), Figs. 2 and 3 and C_s is the heat capacity of Si.

The boundary conditions at all interfaces take into account the heat conduction (Eq. (3a)) and where necessary

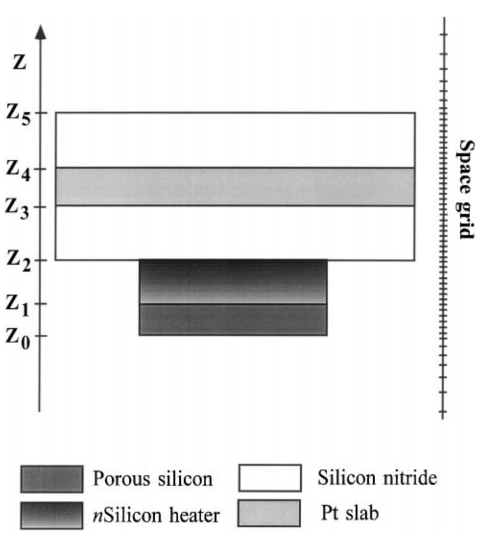

Fig. 2. Longitudinal cross-section of the pellistor.

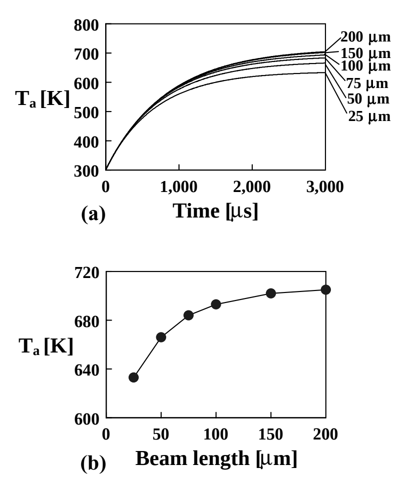

Fig. 4. (a) Average temperature at the pSi/air interface vs. time for different beam length. (b) Average steady-state temperature at the pSi/air interface vs. beam length (power consumption—100 mW, pellistor dimensions—Table 1).

Table 1
Typical dimensions of the pellistor (μm) (Figs. 2 and 3)

A_x	H_x	A_y	H_y	$Z_1 - Z_0$	$Z_2 - Z_1$	$Z_3 - Z_2$	$Z_4 - Z_3$	$Z_5 - Z_4$
300.0	200.0	15.0	10.0	0.5	1.5	0.4	0.2	0.4

Table 2
Physical constants used throughout the simulations valid at 773 K

Material	Thermal diffusivity ($m^2\,s^{-1}$)	Thermal conductivity ($W\,m^{-1}\,K^{-1}$)	Emissivity	Density ($kg\,m^{-3}$)	Heat capacity ($W\,s\,kg^{-1}\,K^{-1}$)
Si	2.204×10^{-5}	45.0	0.5	2.32×10^3	880
Si_3N_4	6.937×10^{-6}	21.0	0.5	3.44×10^3	880
Pt	2.395×10^{-5}	75.0	0.1	2.145×10^4	146
Air	5.564×10^{-5}	4.04×10^{-2}		0.705	1.03×10^3

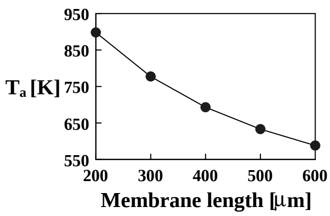

Fig. 5. Average steady-state temperature at the *p*Si/air interface vs. membrane length (power consumption—100 mW, pellistor dimensions—Table 1).

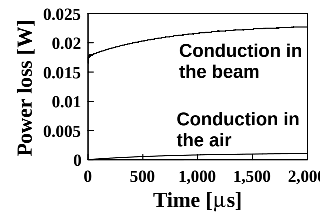

Fig. 7. Energy loss from the membrane due to conduction in the ambient air and conduction into the adjacent supporting beam (power consumption—100 mW, pellistor dimensions—Table 1).

(at all outer surfaces of the pellistor) the heat radiation (Eq. (3b)).

$$k_i \frac{\partial T}{\partial \varphi} = k_j \frac{\partial T}{\partial \varphi} \tag{3a}$$

$$k_i \frac{\partial T}{\partial \varphi} = k_a \frac{\partial T}{\partial \varphi} + \varepsilon_s \sigma (T^4 - T_a^4) \tag{3b}$$

where T_a is the ambient temperature; σ the Stefan–Boltzmann constant ($5.67 \times 10^{-8}\ W\,m^{-2}\,K^{-4}$); ϵ_s the emissivity of Si; k_a, k_i and k_j the thermal conductivities of air and of any other phases of the pellistor, respectively; and $\varphi = X$, Y or Z.

The set of equations of heat transfer (Eq. (1)) for each layer of the pellistor (Fig. 2) and the surrounding air with the appropriate boundary conditions (Eqs. (3a) and (3b)) were solved numerically by the Brian's modification of the implicit alternating-direction finite difference method [3]. A mixed uniform/non-uniform space grid with respect to the Z direction (Fig. 2) was used for reducing the computational time. The region of the highest density of nodes included the membrane and its surrounding. Outside this region the Z spatial increments increased exponentially (Fig. 2). The source code of the program for numerical integration of Eq. (1) was written in ANSI C and was run on a VAX/VMS computer. The program calculated the transient average temperature (T_a) at the porous Si/air interface ($Z = Z_0$, Fig. 2), the heat loss due to conduction and radiation and the temperature distribution at a preselected time. A program in Microsoft C was used to create the data file containing the geometrical dimensions of the pellistor, the three dimensional spatial grid and the physical constants used in the model.

3. Numerical simulations

The geometrical dimensions and the physical constants used throughout the model simulations are given in Tables 1 and 2, respectively. The ambient air temperature was assumed to be 300 K. If not stated otherwise the value of the power consumption used in the calculations is 0.100 W

The beam length was varied in the range from 25 to 200 μm. The corresponding transient average temperature (T_a) at the porous Si/air interface ($Z = Z_0$, Fig. 2) is shown

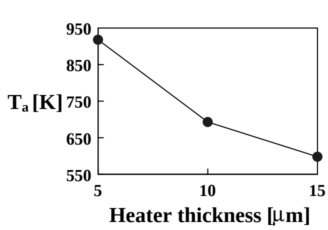

Fig. 6. Average steady-state temperature at the *p*Si/air interface vs. heater width (power consumption—100 mW, pellistor dimensions—Table 1).

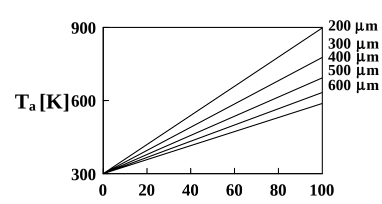

Fig. 8. Average steady-state temperature at the *p*Si/air interface vs. power consumption for different membrane length (power consumption—100 mW, pellistor dimensions—Table 1).

in Fig. 4a. For beam length greater than 100 μm, the increase in the average steady-state temperature becomes insignificant (Fig. 4b) and it can be assumed that 100 μm is the optimal beam length.

The combined thickness of the Pt resistor and the Pt connection ($\Delta Z = Z_4 - Z_3$, Fig. 2) is not expected to exceed 0.2 μm. It was found that variations of ΔZ between 0.1 and 0.2 μm did not affect the thermal performance of the pellistor.

As expected, the numerical simulations showed that the average steady-state temperature increased (Fig. 5) with reducing the membrane length (H_x, Fig. 3).

It was found that by decreasing the heater thickness ($\Delta Z = Z_2 - Z_1$, Fig. 2), the thermal performance of the pellistor could be improved significantly (Fig. 6).

By studying the energy dissipation during the heating of the pellistor, it was found that the heat conduction from the heater into the supporting beams was the main source of heat loss (Fig. 7). The radiation loss was negligible. This result explains the linear dependence of T_a on the power consumption, Q, (Fig. 8) since the only non-linear term with respect to the temperature in the thermal model of the pellistor is the one accounting for radiation (Eq. 3(b)).

4. Conclusions

Considerable improvement in the thermal behaviour of the pellistor outlined above can be achieved by reducing the membrane size (length and width) and the thickness of the heater. The optimal beam length was found to be 100 μm. The thickness of the Pt slab does not influence considerably the thermal behaviour. The main source of heat loss results from heat conduction from the heater into the supporting beams and further improvement of the thermal performance of the pellistor can be achieved by reducing their cross-section.

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References

[1] E. Jones, The pellistor catalytic gas detector, in: P.T. Mosley, B.C. Tofield (Eds.), Solid State Gas Sensors, Adam Hilger, Bristol, 1987 chap. 2.

[2] S.D. Kolev, M. Adam, I. Bársony, A. van den Berg, C. Cobianu, Mathematical modelling of porous silicon based pellistor-type catalytic flammable gas sensors, Microelectronics Journal 29 (4/5) (1998) 235–239.

[3] B. Carnahan, H.A. Luther, J.O. Wilkes, Applied Numerical Methods, Wiley, New York, 1969.