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Quasi Three-Dimensional Simulation of Heat Transport in Thermal-Based Microsensors

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Abstract

Results based on quasi three-dimensional numerical solutions of electrothermal behaviour in thermally isolated microstructures are presented. Here, we solved the two-dimensional system of electrothermal equations with heat loss to the surrounding (due to natural convection) incorporated as a mixed boundary condition. The convective heat loss was calculated based on a three-dimensional solution to the heat conduction equation using a boundary element method. The technique, employed in the analysis of heat transfer in a μ-Pirani gauge, yields numerical soultions which provide good agreement with measurement data.

1. Introduction

Thermal-based microsensors are required in a variety of sensing applications including detection of flow rate [1], pressure (vacuum) [2], and gas species [3]. In flow sensing, the heat loss from a resistively heated microstructure (due to forced convection) is modulated by the flow rate. In gas sensing, an isothermal heat surface (microhotplate) can be used to raise the temperature of the sensing film to increase absorption or reaction of gas on the film surface. With pressure sensing (based on the Pirani principle), heat transfer from a heating element is modulated by the mean free scattering length of molecules (or gas thermal conductance) which is pressure-dependent.

For insight into device operation including underlying heat transport mechanisms and for optimization of device design to meet key requirements of fast response time, low operating power and temperature, fast thermal response, it is necessary to solve the coupled system of equations governing electrothermal behaviour. Of particular importance in all of the above applications, is the modeling of heat loss from the microstructure to the ambient. For example, with the microstructure we have considered here (see Figs. 1 and 2), the heat loss due to natural convection can be as much as 99% of the input power at standard temperature and pressure (STP) [4]. Thus accurate modeling of the boundary condition accounting for the convective heat loss is crucial in a two-dimensional simulation.

2. Assumptions, Model Equations, and Numerical Procedure

In view of the planar nature of thermally isolated microstructures and because of small film thicknesses (relative to other linear dimensions), the electrothermal behaviour within the structure can be adequately described in two-dimensions. The approximation, although reasonable in terms of electrical behaviour, may not be intuitively obvious from a thermal standpoint and requires justification. In most structures, under conditions of natural convection in the diffusive limit (i.e. stagnant fluids), the Biot number is relatively small; this number describes the ratio of the surface heat conductance to the internal heat conductance across the microstructure thickness. Measurements performed on heat transfer test structures show that the gradient across the thickness at STP is negligible compared to the lateral gradients [5]. Given these conditions, electrical and heat transport within the microstructure can be described by the following 2-D system:

$$\nabla_{x,y} \cdot [\sigma(T)\, \nabla_{x,y}\, \psi] = 0 \tag{1}$$

$$\nabla_{x,y} \cdot [\kappa(T)\, \mathrm{grad}\, T] = \sigma(T)\, (\nabla_{x,y}\, \psi)^2. \tag{2}$$

Here, $\sigma(T)$ denotes the temperature-dependent electrical conductivity of the polysilicon regions (see Fig. 2), ψ is the electric potential, $\kappa(T)$ is the temperature-dependent thermal conductivity, and T is the temperature. The term on the right-hand-side of eqn. (2) denotes Joule heat.

In the presence of a flow stream, the steady-state heat transport from the surface of the microstructure, assuming negligible viscous dissipation, is governed by the energy equation:

$$\rho C_p\, [u\, \partial T/\partial x + v\, \partial T/\partial y + w\, \partial T/\partial z] = \nabla .\, (\kappa(T)\, \nabla\, T) \tag{3}$$

where u, v, and w are the components of the velocity field, ρ is the density, and C_p is the specific heat. With zero flow, we can assume that the natural convective currents are negligible. Despite the excessively high ($\approx$ 400 °C) in-situ heated temperatures, the resulting Grashof number, which describes the ratio of buoyancy to viscous fluid forces, is small. Measurements show that the heat loss from such microstructures is independent of its orientation with respect to the gravity vector [5]. Thus we can assume that the fluid is stagnant (diffusive) and that the temperature distribution obeys $\nabla .\, (\kappa(T)\, \nabla\, T) = 0$ where $\kappa(T)$ denotes the thermal conductivity of the fluid expanse (air) and is pressure-dependent. For given surface temperature of the microstructure, $T_s(x,y)$, the temperature of the micromachined cavity walls, and the temperature of the fluid far from the microstructure surface (free stream temperature, T_∞), the equation can be solved to determine the convective heat loss from the microstructure surface to the surrounding [5]. This heat loss constitutes the boundary condition required for eqn. (2). The technique to solve this equation is based on a boundary element method along the lines reported in [6]. However, it can be reduced to Laplace's equation by employing Kirchoff transformation and this intrinsically accounts for the temperature dependence of the thermal conductivity [7]. Based on the solution, we calculate a heat transfer function $G(x,y)/(\kappa°C)$ on the membrane surface. The surface heat density at position (x,y) on the membrane surface

$$q_s = \kappa\, G(x,y)\, [T_s(x,y) - T_\infty] \tag{4}$$

is then employed as a mixed boundary condition for the two-dimensional solution of eqn. (2). Since the heat transfer function G(x,y) is a function of $T_s(x,y)$, it is recalculated within the iterative loop used in the solution of eqns. (1) and (2). Radiative heat losses, if necessary, can also be incorporated as a mixed boundary condition. In our case, in view of the given device active area and input powers involved, such losses are negligible.

Equations (1) and (2) are discretized using a control area approximation with node count of 1600 and 4700, respectively, for the structure shown in Fig. 1. The procedure starts with the calculation of G(x,y), following which a system of equations for the electrical conduction equation is generated. Based on the solution, the Joule heat terms are calculated and eqn. (2) is solved. Since (2) can be potentially nonlinear, an inner iterative loop is employed. The solution of the systems of equations is based on a conjugate gradient scheme. Solution verification is based on electrical and heat flux conservation checks.

3. Results and Discussion

The simulated temperature distribution in the device (see Figs. 1and 2) in air at STP is illustrated in Fig. 3. The peaks and valleys correspond to the temperature distribution of the active (current carrying) and passive (temperature sensing) coils, respectively. The thermal behaviour of both coils was measured for both air and helium at STP. The temperature values shown were based on measurements of coil resistance from which an average coil temperature is retrieved following prior temperature coefficient characterization of the polysilicon layer. The temperature difference between active (T_{ac}) and passive coils is illustrated in Fig. 4 as a function of the input power. With maintaining the active coil average temperature at 70°C, we clearly see that the input power (heat loss) is consistent with the thermal conductivities of the two gases implying an almost 100% transduction efficiency. The larger temperature difference in the case of helium is due to the convective heat loss to the surrounding which predominates over the inter-coil lateral heat transfer.

4. Conclusions

In this paper, we have presented the necessary assumptions, resulting model equations, and boundary conditions pertinent to two-dimensional numerical simulation of heat transport in thermal-based microsensors taking into account convective heat losses. The simulations provide good agreement with measurement data.

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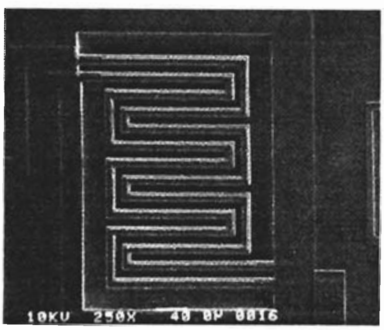

Fig. 1 Photomicrograph of device used in simulations.

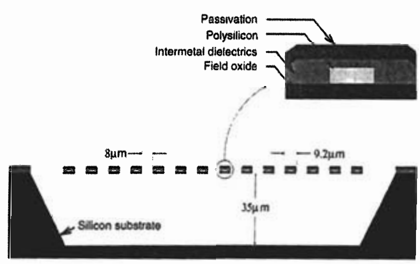

Fig. 2 Device cross-section.

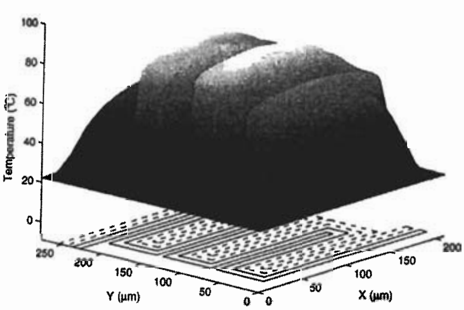

Fig. 3 Temperature distribution in device at STP (dashed line: active coil, solid line: passive coil).

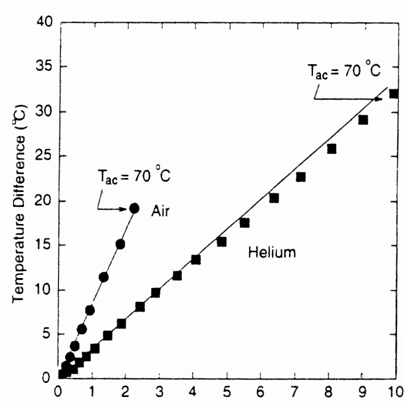

Fig. 4 Temperature difference between coils as a function of input power (solid lines: simulations, points: measured values)