Multiphysics FEM Simulations Approach for Development of MEMS Heat Generator

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Abstract: Design and computing simulation, fabrication and characterization of a thin film Ti/Pt heater evaporated on a Silicon substrate and integrated with a microfluidic is presented. The heater was integrated with a microfluidic system obtained with classical photolithography process consisting in a polydimethylsiloxane (PDMS) stamp. Before realizing the heater the heat transfer of system with external environment was simulated for a following comparison with the real device. Models have been developed using COMSOL Multiphysics incorporated in a optimization routine to study and predict the behaviour of microheater made with metallic resistor over a Silicon surface with the goal to developing a tool that can be used to design different geometrical configurations with different materials. The simulation results, and as consequence the model, were found to be adequate to present the behaviour of microheater and the heat transfer with microfluidic system. The model can be used to compare different geometrical configurations and the thermal behaviour of different materials.

Keywords: Microfluidics, MEMS, Microheater.

1. Introduction

Accurate fluid temperature control in microfluidic channels is a requirement for many lab-on-chip and micro-reactors, especially in biotechnology and in chemistry where most process are highly temperature sensitive [1]. Frequent applications utilize precise, controlled and localized heating to enable the required process taking place in microchamber closely coupled to the heating source. Micro-reactors for hydrogen production in fuel cell applications are a good example of such application [2,3]. Another example of possible application of micro-heaters is the gas pre-concentrator integrated in a micro gas chromatograph. Here, in particular high thermal dynamics, uniformity and high surface area to volume ratio are required [4,5]. Before realising a new microdevice it is important to predict how this system will operates, under what physical or chemical condition, in order to optimize the realisation time, the cost of materials and to understand what are the limit of device. To do this, the finite element analysis is a nice tool to evaluate the characteristics of a system. Finite element analysis (FEA) has become commonplace in recent years, numerical solutions to even very complicated stress problems can now be obtained routinely using FEA. In this work we have designed and developed a microfluidic system based on a single channel integrated with a Ti/Pt micro-heater useful for biosensors applications. The fabrication of microfluidics device is based on standard photolithography techniques for master realization [6, 7, 8, 9]. Thin films resistive metal heaters have proven to be the best choice for localizing heating applications with integrated microfluidics systems. In our case, Platinum thin layer has been used as metal to realise the meander because it exhibits a positive and linear temperature dependence. Other optimal characteristics of Platinum for these applications are an excellent long–term stability, chemical inertness, a well-established manufacturing processes and good mechanical properties. In order to guarantee a good adhesion, a thin layer of Ti (50nm thick) was deposited between Platinum and Silicon substrate. The goal of this work is the modelling, design and fabrication of a microfluidic system integrated with Ti/Pt film microheater to control the temperature ranging between 20°C-130°C potentially useful in liquid phase optical sensing application.

2.Theoretical model and numerical simulation

Before the practical realisation of the microchannel with integrated heater, a theoretical analysis and computer simulation has been performed in order to understand the effect of heat transfer from the Platinum/Titanium meander to liquid by Joule heating effect. The calculations was based on finite element method (FEM) and carried out by using COMSOL Multiphysics 4.2a. In this paper the theoretical analysis was performed by using three different models, in the first one the heat transfer inside materials of Pt/Ti microheater was analysed; the laminar flow model was used to study the fluid dynamics inside the micro-channel. In the simulation process the temperature of the inlet fluid was set at room temperature value and the coupling with heat transfer model permitted us to verify the increase of fluid temperature at outflow. With the third model we studied mechanical deformation of materials caused by thermal stress. Every simulation ran in stationary mode

2.1 Heat transfer

In order to simulate the controlled heat transfer onto a specific substrate a suitable Ti/Pt metallic resistance was designed by considering two experimental configuration: Silicon substrates with and without PDMS channel. In order to obtain realistic results the convective cooling with environment was considered, so an external natural convection from the meander surface having a geometrical ratio A/p (where A is the area covered form the meander and p the meander perimeter) equal to 1.46 mm was imposed. Here the dry-air as external fluid with a pressure of 1 atm and an external temperature of 20°C was hypothesized. A thickness of the meander of 300nm was used as parameter.

The same convective cool condition was imposed also for Silicon and on Silica glass surfaces, using in particular as geometrical parameters 0.1 mm for height and 5.93 mm for the ratio A/p of Silicon and 1mm as height and 2.29mm as ratio A/p for Silica glass support.

Here a 3D heat conduction model to describe the problem was used governed from the equation:

$$\rho C_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right) + Q \quad (1)$$

where ρ is the density of the medium, C_p is the specific heat of the medium, T is the absolute temperature of the medium, k is the conductivity of the medium and Q is the heat source.

In this case the heat source Q is obtained by means of Joule effect and the power consumption is given by equation:

$$Q = I^2 R = \frac{V^2}{R} \quad (2)$$

where I is the current that flows in the resistance R and V is the voltage applied.

In this work a free triangular mesh set as extremely fine on surface of Ti/Pt meander resistance and a swept condition on vertical wall was used; in particular, for Silicon, Silica Glass and PDMS surfaces the mesh used was always a triangular mesh, but set as normal .

2.2 Fluid Flow

The flow of an incompressible Newtonian liquid in microchannels can be described by continuity equation and Navier-Stokes equation [10] as shown in equations (3),

$$\nabla \cdot \vec{V} = 0$$
$$\frac{\partial \vec{V}}{\partial t} + \vec{V} \bullet \nabla \vec{V} = -\frac{1}{\rho}\nabla p + \mu \nabla^2 \vec{V} \quad (3)$$

where $\vec{V}$ is the velocity vector, p is the pressure, ρ the density and μ is the kinematic viscosity of the fluid.

From the fundamental theory of fluid dynamics, three regimes of the flow exist, which are characterized by a dimensionless parameter known as the Reynolds number, Re. It is expressed by the following equation,

$$\mathrm{Re} = \frac{Vd}{\mu} \quad (4)$$

where V is the mean flow velocity of the fluid and d is the characteristic length of the flow.

For fluid moving in a closed channel, the hydraulic diameter of the channel is often used as characteristic length in computation of the Reynolds number. If the Reynolds number is less than 2300 the flow is considered in laminar regime, if the Reynolds number ranging between 2330 and 4000 the flow is considered in transitional regime. If the Reynolds number exceeds 4000 the flow is considered in turbulent regime.

The Reynolds number in microchannels rarely exceeds 2000 for moderate pressure of 1-10bar so in microchannels the flow is considered in laminar regime and this is the assumption that we made in our simulation model [11].

The two models (fluid dynamic and heat transfer models) were coupled imposing that the fluid temperature at outflow was that produced by heat transfer model.

2.3 Resistor and thermal stress

The temperature profile can be used to determine the stress-strain of the materials and thermal expansion. If the stress is above the ultimate stress of the material then it will break. The stress can be described through the following equation

$$-\nabla \bullet \sigma = \vec{F} \quad (5)$$

where $\vec{F}$ is the body force and σ is the stress tensor. The stress-strain relationship is given by equation

$$\sigma = \vec{D}\varepsilon \quad (6)$$

where $\vec{D}$ is the elasticity matrix. The symmetry plane is constrained in the normal direction, and the boundary where the voltage is applied is constrained from moving in the x, y or z directions. This allows the resistor to move up or down in z-direction.

The thermal stress analysis was used to study mechanical deformations of PDMS to evaluate channel's deformations with consequent occlusion of the same and the loss of adhesion between PDMS and Silicon surface.

3. Experimental details

3.1 Fabrication procedure of micro-heater

Titanium/Platinum (Ti/Pt) heater element was realised through conventional photolithography. The heater element was fabricated with electron beam evaporation of Platinum thin films on Silicon substrate (3x 3cm^2). The substrate was cleaned with the Piranha solution (H_2SO_4+H_2O) for 20 minutes, washed with deionized water to 18 Mohm, dried with N_2 and after put on a hot plate at 200°C for 30 minutes. A positive resist (AR-P5350 Allresist) was spun on the Silicon substrate at 500 rpm for 5 seconds and after at 4000 rpm for 30 seconds. Then the sample was put on a hot plate at 110°C for 5 minutes. For the exposition step, an heated mask (made in chromed quartz) was aligned with the sample and an UV radiation with the wavelength range 350-500 nm was used for 10,5 seconds. The resist was developed with developer AR 300-26 diluted with water with ratio 1:25 for 25 seconds, then washed with deionised water to 18 Mohm and dried with N_2. The micro-heater was evaporated onto Silicon surface by electron beam evaporation.

The evaporation process required two steps, the evaporation of Titanium layer and the evaporation of Platinum thin film. For Titanium evaporation the pressure chamber was in a range among 10-6 mbar, with a filament current of 18 A and an emission current of 50 mA. The deposition time was 15 seconds. For Platinum evaporation the pressure chamber was the same of process for Titanium evaporation, but the filament current and the emission current were 20 A and 160 mA. The deposition time for Platinum was 4 minutes and 3 seconds. The power supply for this operation is a high voltage D.C. power supply. The voltage applied for our evaporations was 11,5 KV for both process. The final height of micro-heater was 300 nm and occupies a surface of 5 x 7 mm^2.

3.2 Fabrication procedure of the microfluidic system

The microfluidics channel was fabricated in PDMS using the soft lithography technique. The master containing the microchannel was fabricated spun on Silicon substrate a layer of SU8 AZ2010 at 500 rpm for 5 seconds and after at 1000 rpm for 40 seconds. Then the wafer was soft baked on two different hot plate at 65°C for 1minute and at 95°C for 3minutes. After the soft bake the wafer was exposed for 12 minutes with a UV radiation with the wavelength range 350-500 nm. The wafer was then post exposure baked for 1minute at 65°C and at 95°C for 3 minutes on two different hot plates. The sample was then allowed to cool to room temperature and developed in SU8 developer, once developed the sample was blown dry with nitrogen. The PDMS (Sylgard 184, Dow Corning) replica was fabricated using prepolymer mixed with current agent in 10:1 ratio, than the mixture were poured onto the wafer and thermally cured at 140°C for 15 minutes. A square of cured PDMS was exposed in a O_2 plasma for 1 minute at 25 W and embedded together with Silicon with heater evaporated on surface. A second plasma treatment was made with same parameters to create a bonding between the microfluidic system and the PDMS sealed on Silcone wafer.

The circuit containing the heater integrated with microfluidic system was connected to a piezoelectric micropump (Bartels Mikrotechnik mp5) and a power generator (Bartels Mikrotechnik) controlled via software realized by using LabView platform (National Instruments Inc.).

4. Simulations and experimental results comparison

Figure 1 shows the micro-heater realised onto Silicon substrate and microheater integrated with microfluidics system and realized with CAD tools.

Figure 1. Optical microscope images of Ti/Pt microheater realised onto silicon substrate, the surface covered is (5x7) mm^2 and CAD rendering of device.

An infrared (IR) camera (FLIR B20) was used to analyze the temperature variations as a function of the applied voltage and current moving inside the Ti/Pt meander. The infrared camera was connected to a laptop to acquire the thermal distribution onto the device. Thermal analysis was performed with and without the flow of liquid into the micro-channel. In particular, the behaviour of the microdevice was studied before, without PDMS microchannel, and after the realisation of the microfluidic element embedded with the heater to analyze the heat transfer among involved materials with and without the presence of fluid motion in the channel and with controlled velocity.

A comparison with numerical simulations are also reported. The images were acquired applying to the electrodes five different potentials ranging 5 to 30V and a perfect correlation between the simulated thermal distribution and the experimental measured values is evidenced in fig.2.

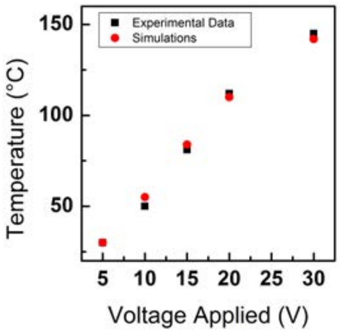

Figure 2. Theoretical and experimental data comparison of the temperature of the microdevice as a function of the voltage applied to the electrodes of the resistance.

The microheater was tested to define a relationship between power consumption and the temperature of the microdevice with and without the presence of a PDMS layer. Experimental measurements put in evidence also higher values of temperature when the microheater is covered with PDMS layer. We stress that the presence of polymer onto the surface of the substrate reduces the heat transfer with environment so the temperature on the surface of device is slightly higher.

As concern the temperature stability of the device, fig. 3 shows a typical measurement at a fixed voltage applied (30 V) to the resistance.

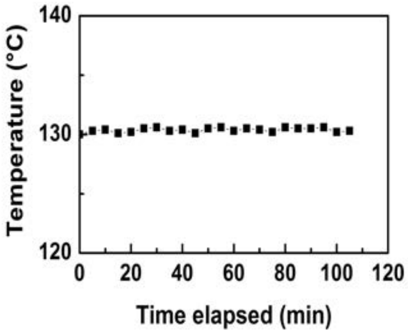

Figure 3. Stability of microheater at max value of temperature (130°C) for 2 hours.

The device remains stable in temperature at a fixed voltage and can run for more than 120 minutes at 130 °C under a fixed power consumption. Fig. 4 is a numerical simulation of thermal transfer in materials of device; in this simulation it's possible to observe an increase of temperature between the inlet and the outlet of channel. At the inlet, the temperature of the fluid is about room temperature, at the outlet there is a thermal gradient of 30°C. From results of computational simulation (Fig. 5) is possible to observe that thermal stress of PDMS, at 10V and with a temperature of 100°C, is 0.016 mm and the mechanical deformation for thermal stress is not significant, so it's possible to observe that the channel doesn't undergo deformation, then the fluid can flows and there aren't hydraulic loss.

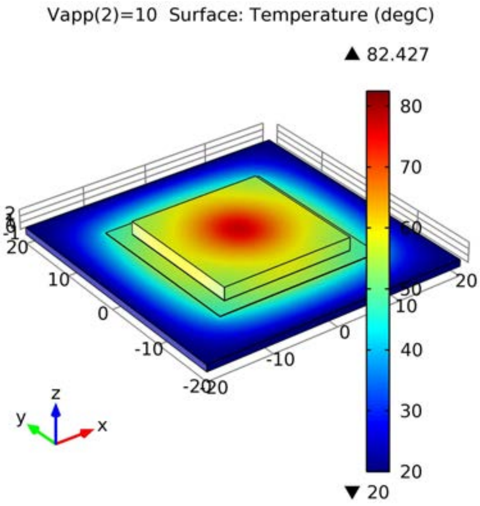

Figure 4. Thermal distribution modelling of microfluidic system integrated with microheater

5. Conclusions

The design, simulation, fabrication and characterization of a miniaturized heater prepared by a Ti/Pt meander deposited onto silicon substrate, integrated with a suitable microchannel useful for microfluidic application is presented. The Ti/Pt meander was fabricated by the combination of photolithographic process and electron beam evaporation, while PDMS microfluidic device was fabricated using booth photolithography and soft lithography. The micro-heater was designed and characterized by using finite elements method to evaluate and calibrate the suitable temperature values as function of power consumption. Good correlation between simulation and experimental data was obtained in the temperature range between 25÷130°C which makes the device very promising for optical biosensing application. The good match between theoretical model and experimental data confirms the applicability of the model to study microheaters behaviour. Modifications of materials and geometries can be made using the explained model which can be used also to optimize the design of heater to reduce energy required for actuation even further. This is an important tool to reduce the time and costs of heater fabrication.

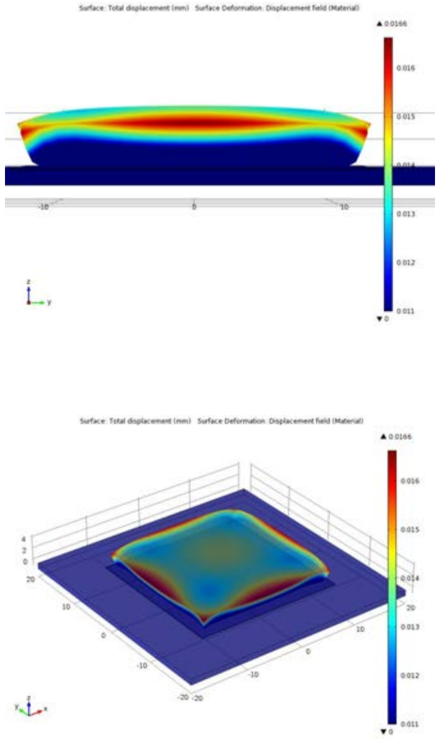

Figure 6. Total displacement of PDMS.

6. References

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