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Finite Element Method-based Design and Simulations of Micro-cantilever Platform for Chemical and Bio-sensing Applications

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ABSTRACT

Micro-electro-mechanical systems (MEMS)-based cantilever platform have capability for the detection of chemical and biological agents. This paper reports about the finite element method (FEM) based design and simulations of MEMS-based piezoresistor cantilever platform to be used for detection of chemical and biological toxic agents. Bulk micromachining technique is adopted for the realisation of the device structure. MEMS piezoresistive biosensing platforms are having potential for a field-based label-free detection of various types of bio-molecules. Using the MEMMECH module of CoventorWare® simulations are performed on the designed model of the device and it is observed that principal stress is maximum along the length (among other dimensions of the micro-cantilever) and remains almost constant for 90 per cent of the length of the micro-cantilever. The dimensions of piezoresistor are optimised and the output voltage vs. stress analysis for various lengths of the piezoresistor is performed using the MEMPZR module of the CoventorWare®.

Keywords: Label-free, bio-sensing, bulk micromachining, micro-cantilever, piezoresistor

1. INTRODUCTION

Development of point-of-care (POC) devices and systems for chemical and biochemical sensing is becoming indispensable need of society. MEMS-based sensors have advantages of miniaturised platform helps in developing portable diagnostic tools. MEMS-based sensors and systems have advantages for the development of ultrasensitive sensors with very low consumption of reagents and analyte, cost effective, better performance, and rapid detection capabilities. Bio-sensors are broadly classified as labelled or label-free sensing platforms[1]. MEMS micro-cantilever-based chemical or biological sensors platform comes under label-free detection system having potential applications for defence and societal needs; these cantilever platforms offer higher sensitivity than other sensing platforms namely quartz-crystal microbalance and surface-acoustic wave based platforms for the detection of chemical agent[2].

Micro-cantilevers are the miniaturised cantilever structures which can be realised using the MEMS technology, viz.; surface micromachining, or bulk micromachining. Each of the techniques has got some advantages and disadvantages. Surface micromachining suffers from the stiction problem and it requires special process like critical point dryer (CPD) to release the structure. Bulk micromachined structures are easy to realise and do not require any special processing tool, but these are larger in size. These micro-cantilevers are very sensitive to detect small change in the mass or surface stress. When these micro-cantilevers are brought in the contact of the gas or analyte, the adsorption takes place and the micro-cantilevers deflect or its resonant frequency changes after the binding of the molecules[3]. Transduction/detection mechanism can be broadly divided into three categories, viz.; optical, piezoelectric, and piezoresistive.

Recently, biochips based on micro-cantilevers have widely been explored for the quantification of transduction of bio-recognition events. Typically, these micro-cantilevers consists of bimaterials like Au and Si beams, where Au provides the surface for the immobilisation of bio-receptors like proteins, antibody/antigen or nucleic acid interactions. After, the binding of analyte with the receptor surface stress is generated which leads to the deflection proportional to analyte concentration[4,5]. Micro-cantilever based biochips are reported to be used for screening of infectious diseases and detection of chemical and biological warfare agents[6]. Typical sensitivity achieved by different researchers for the micro-cantilever based bio-sensor platform is given in Table 1.

Reports about the design and simulations of a piezoresistive micro-cantilever platform based on CoventorWare®, a commercial finite element analysis (FEA) tool designed specifically for MEMS applications[12]. Placements of polysilicon piezoresistors are crucial and their placement is optimised to measure differential surface stress caused due to adsorption of any bio-molecule on the functionalised layer. Sense and reference micro-cantilevers are connected in a

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Table 1. Sensitivity achieved based on bio-sensor platforms

Biosensor principle /Technique	Transduction /Principle	Limit of detection (surface-stress change)/ Resolution
Micro-cantilever (static mode)[7-10]	Piezoresistive	5×10^{-3} N/m 10 nM 100 fg/ml
	Optical	0.2 ng/ml
Nanomechanical (static mode)[11]	Optical	10 nM

Wheatstone bridge configuration to obtain an output voltage corresponding to the change in resistance of the polysilicon piezoresistors. Piezoresistive detection have advantages over the optical technique, mainly, it does not require expensive optical components and no time consuming laser alignment are needed, also on-chip integration of readout electronics is possible.

The adsorption of any bio-molecule takes place on the functionalised layer of sense micro-cantilever which causes a differential surface stress resulting in the bending of micro-cantilever beam[12,13], which is here detected by the polysilicon piezoresistors. Sense micro-cantilever is connected with the reference micro-cantilever (devoid of functionalisation layer) in a Wheatstone bridge configuration to obtain an output voltage.

2. THEORETICAL DESCRIPTION

The adsorption of bio-molecule on the functionalisation layer produces differential surface stress resulting in the bending of the micro-cantilever beam. The polysilicon piezoresistor placed on the micro-cantilever helps in the transduction of input mechanical signal into the electrical signal owing to its piezoresistive property (i.e.; described by the piezoresistive coefficients of polysilicon). The displacement of micro-cantilever can be measured using the Stoney's Equation (see Equation-1)[14] which is a function of the differential stress.

$$\delta = \frac{3\sigma(1-\upsilon)L^2}{Et^2} \quad (1)$$

where E is the Young's modulus, δ is the displacement, σ is the differential surface stress, υ is the Poisson's ratio, L is the length and t is the thickness of the micro-cantilever.

3. DESIGN AND SIMULATIONS

The dimensions of micro-cantilever are proposed to be 500 µm × 100 µm × 2 µm and a dual-leg polysilicon piezoresistor is mounted on the micro-cantilever to be realised by the bulk micromachining technology.

The micro-cantilever model was designed with the help of different features of CoventorWare®. The sequential flow of device design is

(a) Material properties database is for the physical properties of materials used in designing a micro-cantilever structure;

(b) Process flow editor- the sequential process flow of device fabrication is defined;

(c) 2-d layout- it is used to define the layout of various masks used during the fabrication process.

The final device model designed is as shown in Fig. 1. The micro-cantilever model is composed of several layers of different materials that are depicted in Figs. 2 and 3.

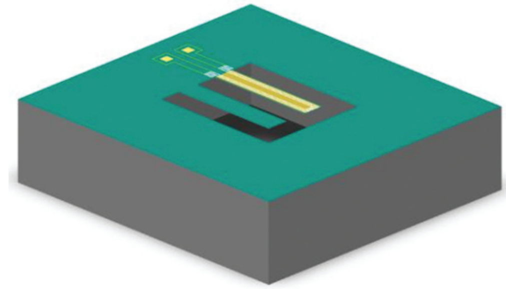

Figure 1. Oblique view of the 3-D solid model.

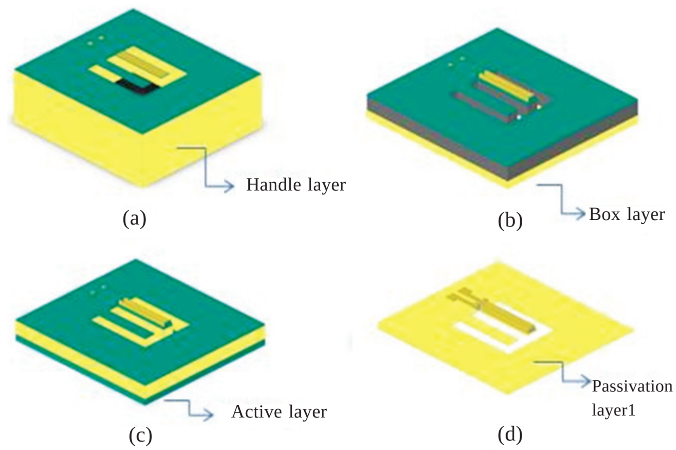

Figure 2. (a) Handle layer, (b) box layer, (c) active layer, (d) passivation layer1.

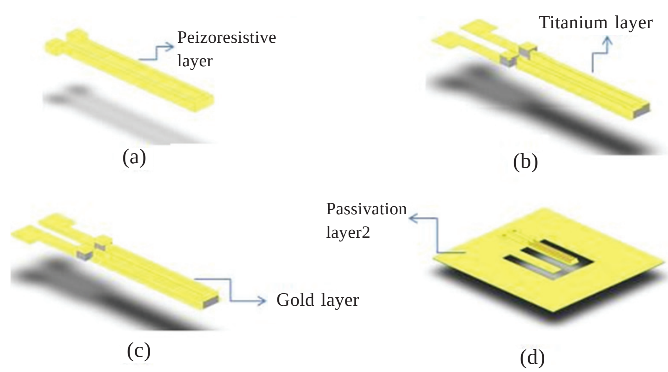

Figure 3. (a) Piezoresistive layer of polysilicon, (b) titanium layer, (c) gold layer, (d) passivation layer².

Finite element method technique is adopted for finding realistic solutions. It uses subdivision of a whole problem domain into simpler parts, called finite elements and encompasses methods for connecting many simple element equations over finite elements, to approximate a more complex equation over a larger domain. The model is divided into finite elements with the help of meshing techniques. The meshing of micro-cantilever is optimised to be of the type extruded bricks, element order to be parabolic, extrude-direction-Z, for obtaining the most accurate results.

4. RESULTS AND DISCUSSION

For the simulations to be carried on the device stress is imparted to the functionalisation layer made of gold and then the transfer of this stress to underlying layers of micro-cantilever and piezoresistor are studied. The MEMMECH module of CoventorWare® helps us in studying the variations of principal stress along the length, width and thickness of the micro-cantilever and piezoresistor (i.e.; mounted on the micro-cantilever). The variation of principal stress 1 (along the length) and principal stress 3 (along the thickness) on the top face of the micro-cantilever is shown in Figs. 4(a) - 4(b).

It is clearly seen that principal stress1 along the length of the cantilever is almost constant and maximum. Stress of magnitude 7.5 MPa is produced on the top face of micro-cantilever (as shown in Fig. 4(a)). The graphs of principal stress3 depict that in micro-cantilever stress varies from (+ve) to (-ve) on going from bottom to top. (as shown in Fig. 4(b)). As we see from the graph that there is a neutral plane (zero stress) at the center of the cantilever. With increase in the thickness of the micro-cantilever, stiffness increases, which intern decreases the sensitivity and resolution.

The sense micro-cantilever is connected with reference micro-cantilever (i.e.; devoid of the functionalisation layer) in a Wheatstone bridge pattern[15] so as to get the output voltage of biosensor in the form of output of Wheatstone bridge. The main aim of taking reference micro-cantilever is to take account of the effect of temperature changes on resistance and to obtain the change in output voltage of bio-sensor completely due to the bio-recognition effect. The output voltage of bio-sensor is measured with the help of MEMPZR module of CoventorWare® for different magnitudes of stress applied to the functionalisation layer. The result is represented graphically in Fig. 5. It is observed from the graph that stress imparted on the functionalisation layer is directly proportional to the output voltage of the bio-sensor.

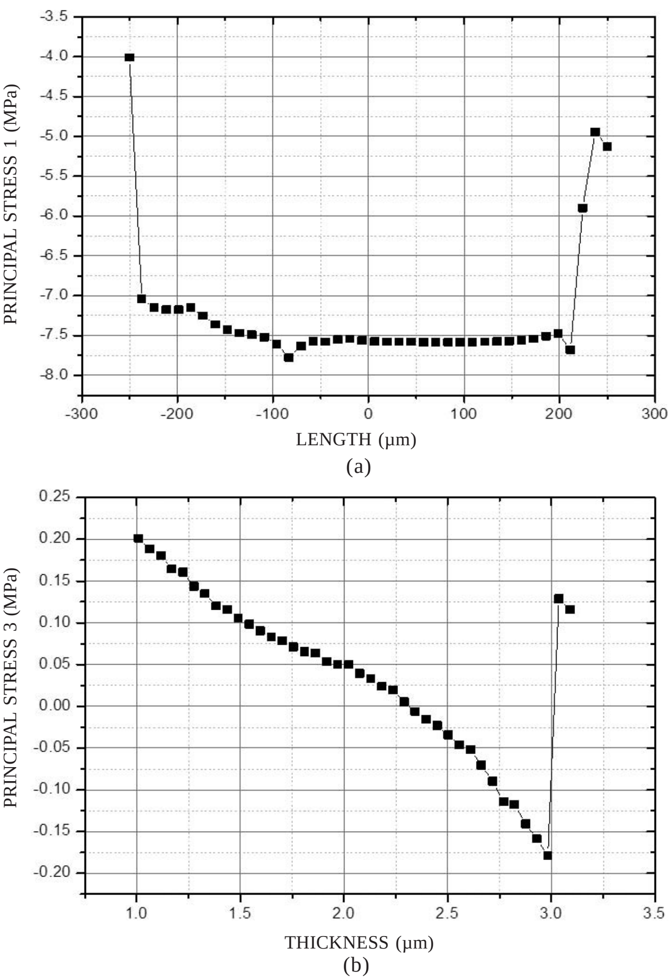

Figure 4. Stress analysis on top face of caentilever (a) Principal Stress 1 (MPa) *vs* Length (μm) and (b) Principal Stress 3 (MPa) *vs* Thickness (μm).

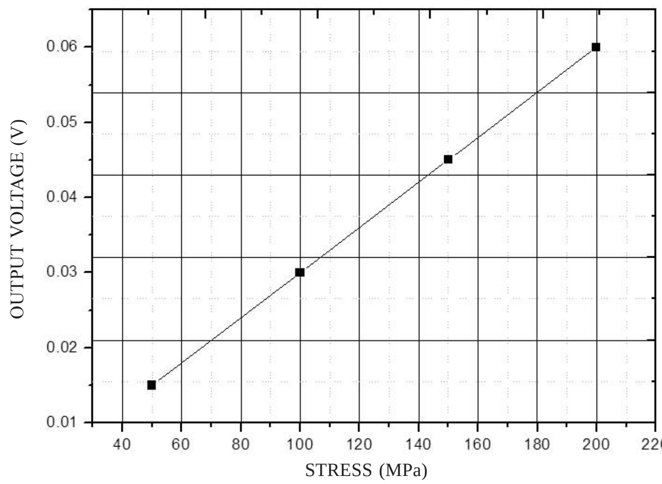

Figure 5. Output voltage (V) *vs* stress (MPa).

5. CONCLUSIONS

In this paper, a micro-cantilever based bio-sensor is proposed and designed to be realised for bulk micromachining technology incorporating label-free detection technique of biosensing. This new cantilever design is different from the conventional design of mechanical sensor from the view point of the position and dimensions of piezoresistor. The mesh optimisations are performed and the stress variations are studied on the surface of micro-cantilever and piezoresistor. According to the stress analysis, piezoresistor should be mounted up to approximately 90 per cent of the length of the micro-cantilever, unlike mechanical sensors. This helps in the maximum transfer of stress induced in the functionalisation layer and hence obtain higher sensitivity of the device and get the output voltage.

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In the current study, his contribution was to design and simulate the micro-cantilever structure for bio-sensing applications.

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In the current study, his contribution was to design masks for the micro-cantilever fabrication for bio-sensing applications.

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In the current study, his contribution was to the biosensors applications of the device and its implementation.

Dr A.K. Goel obtained his MSc and PhD from CCS Haryana Agricultural University, Hisar. Currently working as Scientist 'F' at DRDE, Gwalior. He was conferred several awards including the *AMI Young Scientist Award-1999, DRDO Laboratory Scientist of the Year' award-2004, DRDO Young Scientist Award-2005, DRDO Technology Group Award-2006 & 2015, DBT Overseas Associateship-2008 and DRDO Technology Day Oration Award-2013*. He is presently engaged in development of molecular and immunological systems for bio-threat agents.
In the current study, he formulated the problem along with scientific and technical discussion for the implementation of the device and its applications.