DESIGN of MICRO CANTILEVER BEAM for VAPOUR DETECTION USING COMSOL MULTI PHYSICS SOFTWARE

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Abstract— This paper gives an overview of micro cantilever beam of various shapes and materials for vapour detection. The design of micro cantilever beam, analysis and simulation is done for each shape. The simulation is done using COMSOL Multi physics software using structural mechanics and chemical module. The simulation results of applied force and resulting Eigen frequencies will be analyzed for different beam structures. The vapour analysis is done using flow cell that consists of chemical pillars in surface reactions and deposition process which consists of active layer for adsorbing the reacting species in the laminar flow through the flow cell.

Keyword- Structural mechanics module, chemical module, chemical pillar, COMSOL Multi physics, Cantilever

I. INTRODUCTION

Detection of different vapours plays an important role in the sensor technology in applications like bio-sensing and chemical sensing areas. Micro cantilever is a widely used component in micro system devices which turn out as an outstanding platform for various sensitive sensors in recent years. A cantilever has a rigid end and stress is applied on the free end. A Micro cantilever detects changes in cantilever bending or vibration frequency hence used as physical, chemical or biological sensor [1]. Micro cantilevers have become so popular from past few decades because of high sensitivity, selectivity, ease of fabrication and flexibility of on chip circuits. Due to convenience to regulate, readily adjustable into unified electromechanical system it provides a wide range in industrial applications.

These sensors consist of a receptor which is specialized for a particular chemical or biological target for monitoring the resonant frequency which shifts due to the mass attached to structure. The difference in resonance frequency is correlated to the amount of attached mass or any other type of force acting upon it. Micro cantilever sensors can be used in air, vacuum or liquid. However damping effect in a liquid medium reduces the resonance response of a micro cantilever.[1],[3]. The bending response remains same in liquid medium. Therefore, the practicability of operating a micro cantilever in a solution with high sensitivity provides an ideal platform to use as chemical sensors and biosensors. These cantilever sensors provides better dynamic response, reduced size and high accuracy, and increased reliability compared to the common sensors.[4],[12].

This paper gives details about the finite element method (FEM) to attain the accurate performance of micro cantilever sensor of different materials that includes Poly Si, SiO_2 and Si_3N_4 of different structures. Analytical calculations and simulation using finite element method (FEM) have been carried out for various shapes and geometries of the cantilever. COMSOL Multi physics, a tool for MEMS to analyse finite element was used to develop a model of the cantilever beams. Also chemical pillars are utilized for the vapours analysis and is designed using the chemical module in COMSOL multi physics.

The micro cantilever of different structures and different materials are studied using the Eigen frequency study in COMSOL Multi physics. Here chemical pillars are utilized for the vapour analysis and is designed using the chemical module in COMSOL Multi physics.

II. LITERATURE REVIEW

For chemical performance, cantilever beams are coated directly by samples or sensor layers and then it exposed to analyte vapours. The shift in bending (static mode) and resonant frequency (dynamic mode) of the micro cantilever beam is measured by various ways. Most commonly methods used before with high accuracy are optical reflection, piezoresistive, capacitance and piezoelectric methods. The advantage of using these techniques is that we can measure both frequency and bending in a single measurement. Different techniques used include

A. Optical Beam Deflection

This is the easiest method to measure the deflection of a cantilever beam. In this method a laser diode is focused at the free end of cantilever. By using position sensing detector reflected beam is examined. Displacement up to 0.1nm can be measured by this technique.[12].

B. Capacitance Measurement Technique

The deflection of the cantilever beam is measured by monitoring the change in capacitance between micro cantilever and fixed electrode. The capacitance changes accurately as a function of cantilever bending. However this method is not suitable in liquid medium.[8],[2].

C. Piezoelectric Technique

This technique utilizes the property of piezoelectric. The surface of cantilever is coated with a thin layer of piezoelectric material. This layer produces transient charges due to movement of cantilever beam. The disadvantage of this technique is it require electrode to piezoelectric film. This technique is generally used in dynamic mode of cantilever beam.[4],[17].

D. Piezoresistance Technique

In this technique the change in resistivity is monitored when stress is applied on the cantilever beam. The layer of piezoelectric material is placed on cantilever beam and it show variation in resistance when cantilever is stressed with the deflection. Deflection can be induced by making changes in the adsorption-induced stress or by thermal stress. The variation in resistance can be measured by using an external dc biased, Wheatstone bridge. The disadvantage of this method is that cantilever should be given with passing current throughout which creates electric noises and thermal drift in micro cantilever deflection.[5],[7].

Earlier methods of vapour detection include using quartz crystal microbalance. Here alkane thiols formed monolayers over the quartz crystal microbalance. The organic vapours interacted with monolayer's by hydrogen bonding and dipole dipole interaction producing mass changes .As such resonant frequency shift can be used to measure mass changes.

Another method included using cantilever based on piezoresistive arsenic sensor wherein the cantilever is coated with arsenic adsorbent. As such the sensing cantilever changes its resistance upon interaction with arsenic particles.

III. DETAILED PROBLEM DEFINITION

Cantilever beams of different shapes and different materials are studied using the eigen frequency study. The different cantilever beam structures are analysed to find out the most suitable one. For this the different beams are subjected to the same mechanical force and the corresponding displacements and eigen frequencies are analysed for each one.

The chemical module design is the second part where the reaction between the analyte vapour and the cantilever sensing layer takes place. The sensing layer material is of importance. Here chemical pillars are utilized for the chemical sensing purpose which consists of active surfaces for adsorbing the chemical analytes.

IV. SOLUTION METHODOLOGY

A. *Micro cantilever beam design*

It is a mechanical structure rigid at one end and a free end that moves when acted upon by a stress. The cantilever acts as a sensor by detecting the cantilever bending as well as the changes in vibration frequency. The cantilever is usually coated with a sensing layer over which the vapour analyte reacts by a lock key mechanism the different cantilever structures include the T shaped, pie shaped, triangular and rectangular cantilever beam. The structure as well as the material used for the design is an important parameter to determine the beam stiffness. The different beam structures is analysed for the same force applied.[1],[16],[17].

B. *Chemical module design*

It is in the chemical module where the interaction between the analyte vapour and the sensing layer occur. This chemical module is mounted over the cantilever beam. The chemical module usually used is a flow cell. The flow cell contains many reacting pillars on it. This pillars are usually concaved shaped and are coated with a sensing material that reacts with the analyte vapour. The analyte is selectively adsorbed on the pillar from the sample stream. Upon reacting with the analyte a signal is produced corresponding to the local concentration.

V. DETAILS OF EXPERIMENT

A. *Micro cantilever Beam Design*

Micro cantilever beams of different shapes rectangular, T shaped and U shaped are designed using COMSOL Multi physics. For modelling the structures, 3 D structure is selected, linear elastic model in structural mechanics is selected and Eigen frequency study is included. Beam of the respective dimension mentioned in the table below is modelled. Different materials like Poly Si, SiO_2 and Si3N4. The study is computed to determine the different Eigen frequencies for different modes of operation.[13],[]14].

TABLE I
Beam Dimension

Beam Dimension	**Value**
Beam length	60 µm
Beam width	10 µm
Beam height	1.4 µm

B. *Chemical Flow cell Design*

Different physics involved in the design of chemical pillars include transport of diluted species, surface reactions and laminar flow of species. Transport of diluted species is used to compute the concentration of solute in the solvent. Mass transport in the analyte stream is given by

$$\frac{\partial Cp}{\partial t} + \nabla.(-Dp\nabla Cp) + u.\nabla Cp = 0$$

Where, Dp denotes the diffusion coefficient Cp the species coefficient and u is the velocity vector

For detection of the analytes, reacting pillars are modeled with the help of chemical module in COMSOL. Here the flow cell in chemical module is used.

The flow cell consists of four pillars arranged in seven rows. Analyte species can be adsorbed and desorbed from the reacting surface according to the following equation

$$P + S \underset{kdes}{\overset{kads}{\Longleftrightarrow}} PS$$

Adsorbed analyte (PS) can transform to a quenched state (QS) that won't contribute to sensor signal and is governed by the following reaction

$$PS \underset{k_2}{\overset{k_1}{\Longleftrightarrow}} QS$$

Rate of adsorption is given using the following equation

$$r_{ads} = k_{ads}Cp$$

Where, c_P is the concentration of P in the stream k_{ads} is the rate constant of adsorption k_{des} is the rate constant of desorption.

The desorption rate is given by

$$r_{des} = k_{des}Cps$$

Where, c_{PS} is the concentration of surface adsorbed species

The sample pulse that enters the flow cell is described using Gaussian distribution with a maximum concentration of 80 mol/m^3 at the flow inlet.

The outlet flow condition is given by

$$n(-D\nabla C) = 0$$

The net flux at the boundaries is

$$N_p = -r_{ads} + r_{des}$$

Surface reaction is used to study the chemical reactions between the surface and bulk species on boundary. Surface species are transported tangentially as per Ficks law and bulk species are assumed to be immobile. Fick's law defines the relation between the diffusion flux and diffusion coefficient. According to the law the flux goes from region of higher concentration to region of lower concentration with the flux proportional to the diffusion coefficient and the negative of the concentration gradient. It is defined mathematically as,

$$J = -D\left(\frac{\partial \phi}{\partial x}\right)$$

Where, J is the diffusion flux

D is the diffusion coefficient or diffusivity and

ϕ is the concentration of the species and x is the position.

The absorbed species travel tangentially along the surface with the surface molar flux as

$$N_{t,i} = -D_{s,i}\nabla_{\mathrm{cs,i}}$$

Where, Ds,i is the surface diffusion coefficient for a species i

$$\frac{\partial cs,i}{\partial t} + \nabla\mathrm{t}\left(-\mathrm{D_{s,i}}\nabla\mathrm{t_{cs,i}}\right) = \mathrm{R_{s,i}}$$

Where, Rs,i is the sum of all sources due to surface reaction and adsorption/desorption.

Laminar flow is used to study the pressure and velocity fields of the laminar flow of species and is governed by Navier-Stokes equation. The fluid flow in the flow cell is given by the Navier-Stokes equation as

$$\rho u.\nabla\mathrm{u} = \nabla\left[-\mathrm{pi} + \mathrm{n}(\nabla\mathrm{u} + (\nabla\mathrm{u})^{\mathrm{t}}) - \left(\frac{2\mathrm{n}}{3}\right)(\nabla\mathrm{u})\right]\nabla.(\rho\mathrm{u}) = 0$$

Where, ρ represents density u represents velocity

n represents viscosity and

p represents pressure in the tubes

The pillars near the wall will absorb more compared to the pillars in the centre of the stream and the pillars near wall takes longer time to release absorbed analytes.

VI. RESULTS AND DISCUSSION

From the following table, rectangular shaped micro cantilever beams give maximum deflection for the same load. Load applied to the respective beams is given below in the table. Here the density of the materials vary for different materials which are 2320 kg/m^3 for Poly Si, 2200 kg/m^3 for SiO_2 and 3100 kg/m^3 for Si_3N_4.

TABLE II
Force applied to different beam structures

Beam Structure	APPLIED FORCE (N)
Rectangular	3.02148×10^{-12}
T Shaped	3.02148×10^{-12}
U Shaped	3.02148×10^{-12}

The following figures show the deflections of the different cantilever beam structures for the respective forces. Here the beams are of the same material SiO_2 which has the best material properties suitable for chemical vapour detection.

The figure below shows the mass loading of a rectangular micro cantilever beam for the respective mass which shows the maximum deflection and the eigen frequency

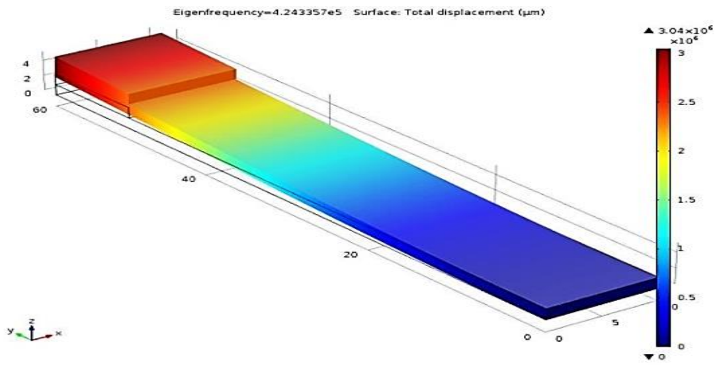

Fig I. Deflection of rectangular cantilever beam

The figure below shows the mass loading of T Shaped microcantilever beam and its respective deflection and eigen frequency

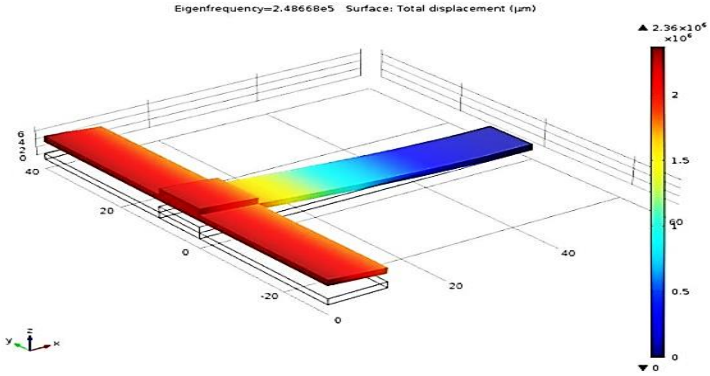

Fig II. Deflection of T Shaped cantilever beam

The figure below shows the mass loading of U Shaped micro cantilever beam and its respective deflection and Eigen frequency.

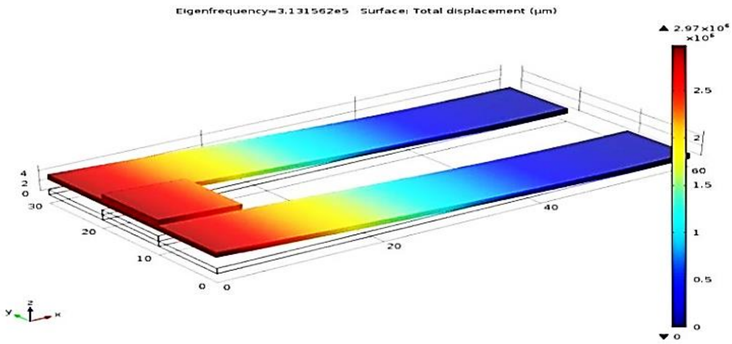

Fig III. Deflection of π Shaped cantilever beam

The following table shows the different eigen frequency values and displacement values for different materials and different beam structures for the same force.

TABLE III
Eigen frequency of beam structures

BEAM STRUCTURE	**EIGEN FREQUENCY (Hz)**			**DISPLACEMENT (µm)**
	Poly Si	SiO_2	Si_3N_4	
Rectangle	4.2433357×10^5	2.87557×10^5	4.5911285×10^5	3.04×10^6
T Shaped	2.408475×10^5	1.631949×10^5	2.605534×10^5	2.36×10^6
U Shaped	3.131562×10^5	2.054559×10^5	3.280743×10^5	3.280743×10^6

The following figure shows the velocity profile of the air molecules adsorbed in the chemical pillars in the laminar flow of water. By changing the diffusivity constant values and rate constant values, different chemical vapor in a fluid flow can be detected. Here the blue regions show the less velocity profiles and the red region shows the maximum velocity profiles. Blue regions represent more adsorbed species near the wall region of the flow cell and red regions shows the unabsorbed species in the laminar flow.

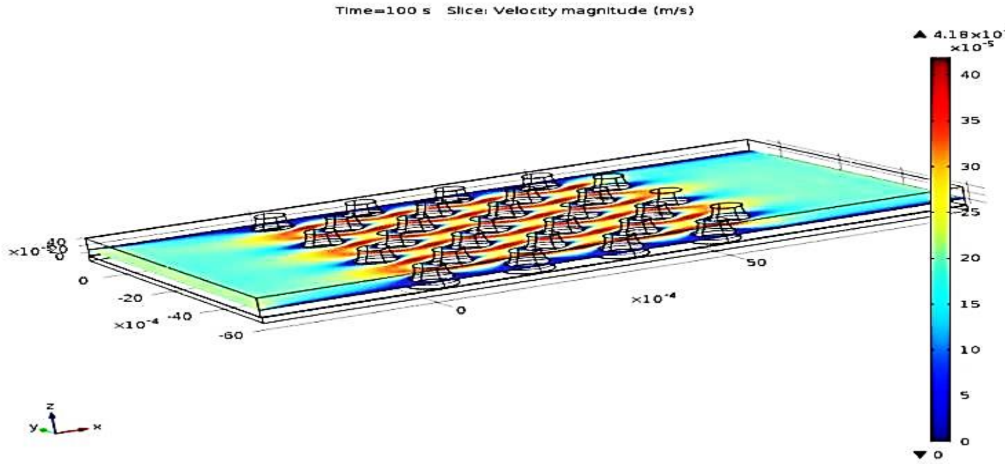

Fig IV. Velocity profile of air molecule

The following figure shows concentration distribution of the laminar flow and surface coverage of adsorbed species at time 45 seconds.[18]

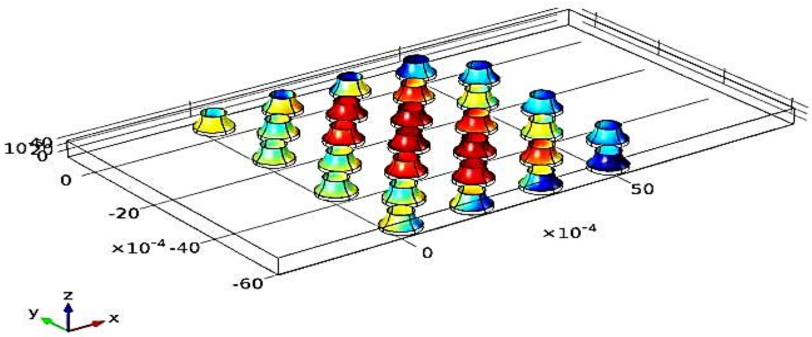

Fig V. Surface coverage of adsorbed species

VII. CONCLUSION

Eigen frequencies of different micro cantilever beam structures are computed using COMSOL Multi physics software. SiO_2 is one of the desirable materials for micro cantilever beams for chemical detection and the different eigen frequencies for different structures includes rectangular shaped beam with a laminar flow*10^5 and U Shaped with a frequency of 2.054559 *10^5 with maximum displacements of 3.04*10^6 µm, 2.36*10^6 µm and 3.280743*10^6 µm for the respective structures. For chemical species detection, chemical pillars are utilized of which different velocity fields are studied using different physics that includes laminar flow, surface reactions and transport of diluted species.

Here the general study of adsorption of air molecules in laminar flow of water is studied. Changing the diffusivity constant and the reaction constant, any combination of chemical vapour and fluid mixture can be studied.

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