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Microcantilever-based Sensors

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ABSTRACT

Micromachined cantilever platform offers an opportunity for the development and mass production of extremely sensitive low-cost sensors for real time *in situ* sensing of many chemical, explosives and biological species. These sensors have been used for measuring and detecting various hazardous chemicals, explosives, and biological agents, leading to the development of hand-held labs. In this paper, different geometries of microcantilevers have been analysed, and their performances in terms of deflection and shift in resonance frequency due to additional mass of analyte have been simulated. The results of these studies can be used to increase the sensitivity of these devices.

Keywords: Sensors, microcantilevers, micromachnied cantilever platforms, detection, hazardous chemicals, explosives chemical sensors, biological sensors.

1. INTRODUCTION

Microcantilever beams are being used for fabricating high performance chemical and biological sensors for detection of explosives like trinitro toluene, and harmful chemical and biological species. These sensors have a wide range of applicability in defence and medical fields[1-6]. These micro-scale sensors utilise a receptor, which is specific to a single chemical or biological target, for immobilising the species of interest and then using a wide variety of physical and chemical mechanisms for detection and transduction, leading to a recordable signal response, as depicted in Fig. 1.

Microcantilever-based sensors have two types of application modes widely used in sensing applications: (a) static mode, where the cantilever bends due to an attached mass or force acting upon it and (b) dynamic mode, where

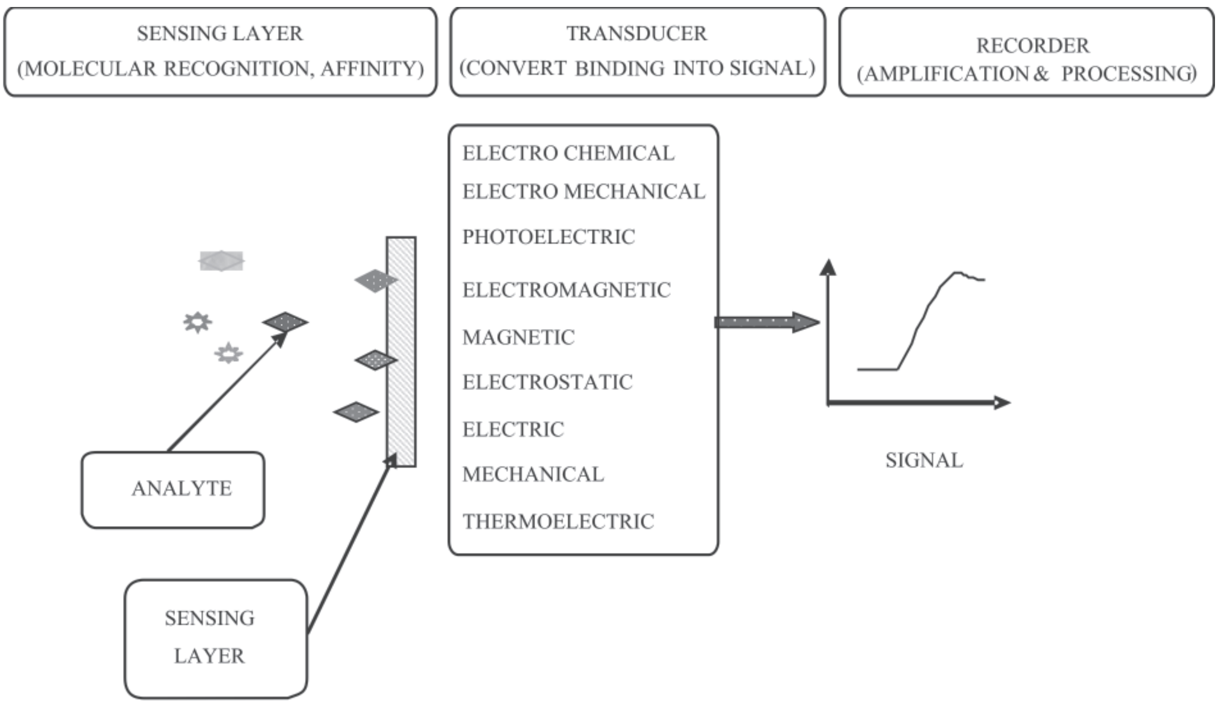

Figure 1. Schematic of general sensor design.

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the resonant frequency is monitored which shifts due to the mass getting attached to the structure. The difference in resonance is correlated to the amount of attached mass or any other type of force acting upon it.

In addition to silicon and polymers, some new materials are also used in these types of sensors. Microcantilever sensors can be operated in air, vacuum or in liquid. The damping effect in a liquid medium, however, reduces the resonance response of a microcantilever. In most liquids, the observed resonance response is approximately an order of magnitude smaller than that in air. The bending response, however, remains unaffected by the presence of a liquid medium. Therefore, the feasibility of operating a microcantilever in a solution with high sensitivity makes the microcantilever an ideal choice for its use as chemical sensors and biosensors. These are the simplest micromechanical systems that can be mass-produced using conventional micromachining techniques. These can be fabricated into multi-element sensor arrays and fully integrated with on-chip electronic circuitry. Therefore, microfabricated cantilevers can provide the basis for a universal platform for real-time, *in situ* measurement and for the determination of physical, chemical, and biochemical properties. These cantilever sensors offer improved dynamic response, greatly reduced size, and high precision, and increased reliability compared to the conventional sensors. As the magnitude of forces involved is very small, increasing the sensitivity of the device is very important. In this paper, basic concept and applications of cantilever beams, detection techniques and device design considerations have been discussed. Analytical calculations and simulation using finite element method (FEM) have been carried out for various shapes and geometries of the cantilever. The results are analysed to improve the device sensitivity.

2. CANTILEVER-BASED SENSING

A cantilever is a simplest mechanical structure, which is clamped at one end and free at the other end. Microcantilever is a microfabricated rectangular bar shaped structure, longer as compared to width, and has a thickness much smaller than its length or width. To serve as a sensor, cantilever has to be coated with a sensing layer, which should be specific, i.e. able to recognise target molecules in key-lock processes. The sensor geometry is shown in Fig. 2.

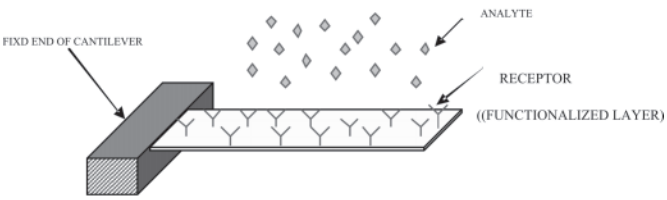

Figure 2. Microcantilever-based biosensor.

Due to the adsorption of target molecules by a sensor, a new molecular layer on the cantilever surface generates the surface stress, and cantilever bends. Adsorption can be controlled by coating one surface of the cantilever with a thin layer of material, which has the affinity towards the analyte. This surface is known as the functionalised surface. Knowledge about the interaction of target molecules with functionalised surface is of great importance as the performance of the sensor depends upon the interaction. This interaction can be physical, chemical or a combination of both. The type of interaction between functionalised molecules and target molecules can cover a wide range, from very strong covalent bond to weak Vander Waals interaction[7].

The other surface of the cantilever (typically lower surface) may be either left uncoated or coated with a passivation layer, i.e. a chemical surface that does not exhibit significant affinity to the molecules in the environment to be detected. To facilitate the establishment of functionalised surface, a metal or polymer layer is often evaporated onto cantilever's surface. Metal surface, e.g. gold, may be used to covalently bind a functional layer that represents the chemical surface sensitive to the molecules to be detected. The gold layer is also favourable for use as a reflecting layer if the bending of the cantilever is read out via an optical beam deflection method. By the functionalisation of the cantilever's surface with different materials, one can use the cantilever in various sensing applications.

2.1 Principle of Operation

Microcantilever sensors can be operated in a air, vacuum or in a liquid. Two commonly used approaches for the operation of cantilever for sensing applications are the adsorption-induced deflection and the resonant frequency shift.

2.1.1 Adsorption-induced Deflection (Static mode)

The continuous bending of a cantilever as a function of molecular coverage with the molecules is referred to as an operation in a static mode. Adsorption of the molecules onto the functional layer generates stress at the interface between the functional and the forming molecular layer[8-10], as shown in Figs 3(a) and 3(b).

The stress is transduced towards the site at which molecules of the functionalised layer are attached to the cantilever surface. Because the force within the functional layer try to keep the distance between molecules constant, the cantilever responds with the bending due to its flexibility.

The resulting surface stress change is calculated according to the Stoney's formula[11] as.

$$\Delta\sigma = Et^2 / [4R(1-\nu)] \quad (1)$$

where, E is the modulus of elasticity, t is thickness of cantilever, R is bending radius of cantilever and v is Poisson's ratio.

The bending of simple rectangular cantilever due to distributed and point loads can be calculated as[12]:

For distributed load

$$\delta = qL^4 / [8EI] \quad (2)$$

For point load

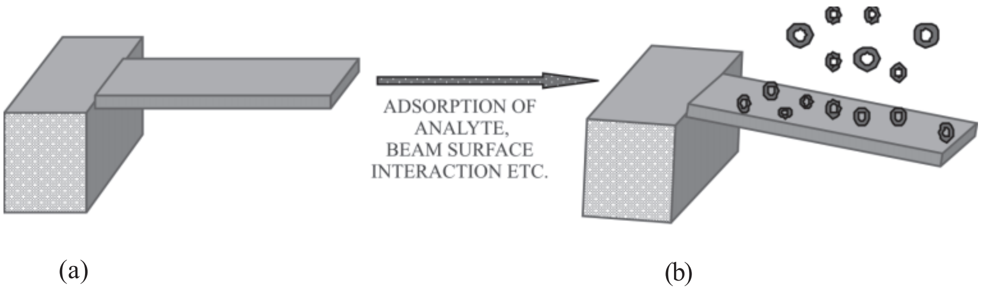

Figure 3. (a) Stress-free cantilever and (b) bending of the cantilever due to the generated surface stress by interaction with analyte.

$$\delta = pL^3 / [3EI] \quad (3)$$

where, d is the deflection, q and p are distributed and point loads, respectively.

The moment of inertia for rectangular cross-sectional beam is given by

$$I = wt^3/12$$

The bending effect of distributed and point loads in case of cantilever that doesn't have uniform area (Fig. 4) can be calculated as:

In case of distributed load, deflection is given by

$$\delta = [q\, L^4/(128EI_1)]\ [1+15I_1/I_2] \quad (4)$$

In case of point load, deflection is given by,

$$\delta = [p\, L^3/(24EI_1)]\ [1+7I_1/I_2] \quad (5)$$

where, I_1 and I_2 are the moment of inertia of different parts of cantilever as shown in Fig. 4.

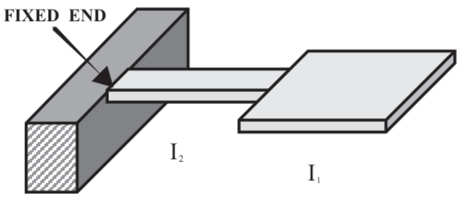

Figure 4. Cantilever with non-uniform area.

This static mode of operation can be performed in various environments. The static mode of operation is ideal in liquid-based applications, however, usually requires rather specific sensing layer, based on molecular recognitions, such as DNA hybridisation or antigen-antibody recognitions.

2.1.2 Resonant Frequency Shift-based Approach (Dynamic mode)

Bending of cantilever is a direct result of the adsorption of the molecules on to the surface of the cantilever. But, here it is rather difficult to obtain the reliable information about the amount of molecules because surface coverage is not known, however mass change can be determined accurately by the resonant frequency shift method. The resonant frequency of oscillating cantilever is given by the formula

$$F = (1/2\pi)\ \sqrt{(K/m^*)} \quad (6)$$

where, K is spring constant and m is effective mass of cantilever.

By adding mass, this frequency shifts towards the lower value and mass change can be calculated. This approach is attractive to sense a small mass but this dynamic mode operation in a liquid environment poses problems such as high damping of cantilever oscillations due to high viscosity of the surrounding media.

2.2 Detection Techniques

The bending and resonant frequency shift of the microcantilever can be measured with high precision using optical reflection, piezoresistive, capacitance and piezoelectric methods. One of the advantages of microcantilever technique is that both bending and resonant frequency can be measured in a single measurement[13]. Various techniques commonly used for detection are:

- *Optical beam deflection*

This is the simplest way to measure microcantilever deflection. In this method, a laser diode is focused at the free end of the microcantilever. The reflected beam is monitored using position-sensing detector (Fig. 6). Displacement of the order of 0.1 nm can be measured by this technique.

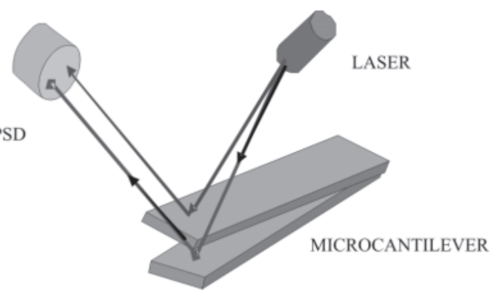

Figure 6. Optical method.

This method has advantages like lack of electrical contacts and compatibility with the liquid medium.

- *Capacitance measurement technique*

This technique of measuring deflection makes use of variation in capacitance between the microcantilever and fixed electrode. The capacitance varies sensitively as a

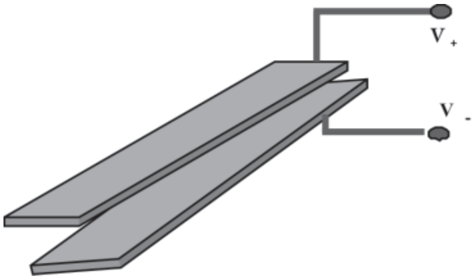

Figure 7. Capacitive method.

function of cantilever bending. However, this technique is not suitable for liquid environment (Fig. 7).

- *Piezoelectric technique*

Piezoelectric technique utilised piezoelectric layer on the surface of the cantilever.Thin layer of piezoelectric material induces transient charge due to cantilever movement. Disadvantage of the piezoelectric technique is that it requires electrodes to piezoelectric film. This method is better suited for the dynamic mode of the cantilever.

- *Piezoresistance technique*

Peizoresistivity is the variation of the bulk resistivity with the applied stress.The resistance of the piezoelectric material on cantilever can change when the cantilever is stressed with the deflection. This deflection can be caused by changes in absorption-induced stress or by thermal stress. The variation in cantilever resistance can be measured using an external dc biased, Wheatstone bridge (Fig. 8). The disadvantage of this method is that it requires passing current through the cantilever. This results in electric noises and thermal drift in microcantilever deflection.

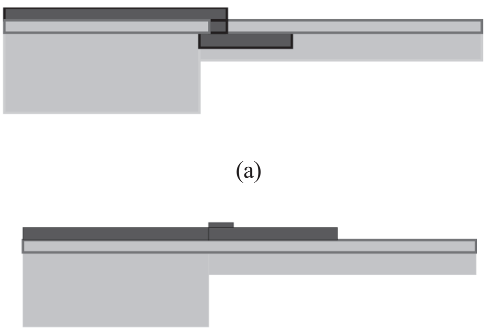

Figure 8. Piezoresistive method; cantilever cross-sections: (a) resistor on the bulk material and (b) resistor on a thin film.

3. DESIGN CONSIDERATIONS

For sensor operation in both static and dynamic modes, dimensions of the structure play an important role[14]. As discussed in section 2.1, deflection, as well as resonant frequency are strongly dependent on sensor geometry. Therefore, different shapes and geometries were studied in addition to commonly employed rectangular geometry to get the maximum sensitivity for a microcantilever-based sensor. Effect of change in the cantilever thickness was also determined. Analytical calculations were done for two types of microcantilever geometries : shape (a) (Fig. 9) is a simple uniform beam having rectangular cross-section, fixed at one end and free at the other end, and shape (b) is a beam with narrow fixed-end and wide at its free-end.

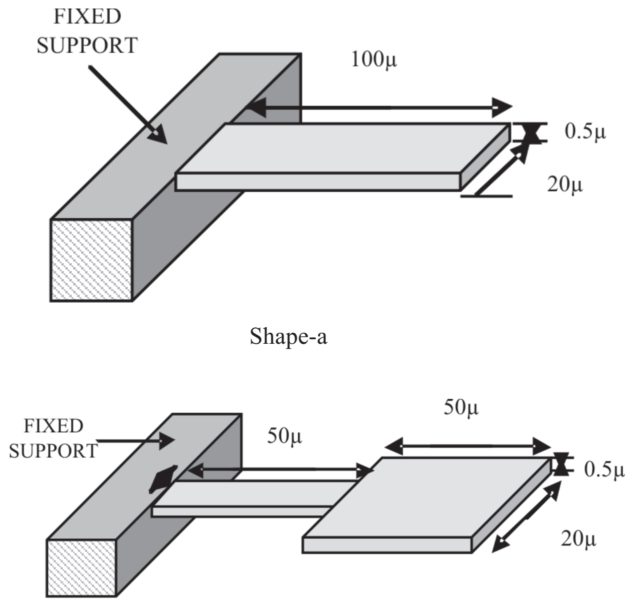

Figure 9. Two types of microcantilever geometries: (a) simple uniform beam fixed at one end and free at the other end, and (b) beam with narrow fixed-end and wide free-end.

Deflection of cantilever was calculated using Eqn (3) for shape-a and Eqn (5) for shape-b. The variation in deflection and resonant frequency were calculated for different values of cantilever thickness. Some more structures, U-shape and V-shape, were also studied as shown in Fig.10.

All the dimensions have been specified in their respective diagrams. The length and the fixed support dimensions are the same in all the structures. Since it is not possible to use analytical modelling for the complicated shapes, FEM was carried out as described in section 4. Only weight as a factor of deformation of microcantilever has been considered in static case.

4. FINITE ELEMENT MODELLING AND SIMULATION

ANSYS Mutiphysics software was used to perform the finite element analysis on different cantilever shapes to determine their sensitivity in both the modes[15]. The solid modelling of all the shapes of microcantilever was carried out using Solid-187 element in the simulation. Solid-187 element was chosen due to support of meshing irregular geometries. In case of static mode, deflection was simulated by applying load to the upper surface of the cantilever. Modal analysis for the determination of natural frequencies

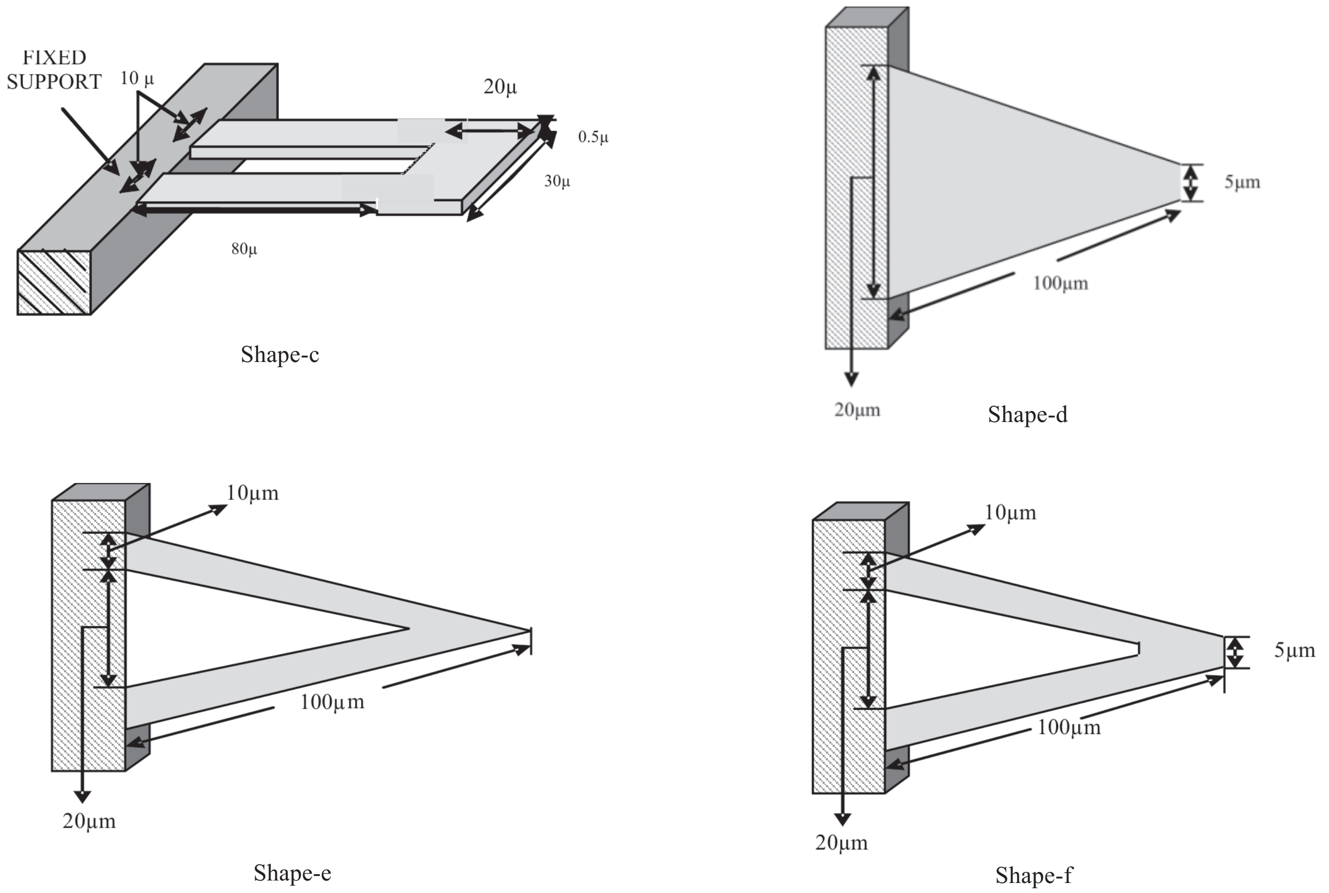

Figure 10. Structured cantilevers with U-shape and V-shape.

was performed by ANSYS. In case of dynamic mode, mass sensitivity was considered the most important parameter for sensing application of very small mass by microcantilever. So frequency shift was calculated by adding a small mass to the cantilever. An amount of 0.232 pg mass was added by attaching a rectangular block of dimensions of 1µm × 1µm × 0.1µm at the upper surface of the cantilever and the resultant change in resonant frequency was simulated.

5. RESULTS AND DISCUSSIONS

In the present work, the FEA of microcantilever in static as well dynamic modes was carried out. For the operation in static mode of the microcantilever, the conventional rectangular shaped cantilever (shape-a) was modelled in ANSYS and deflection was calculated. Deflection was also calculated analytically using Eqn(3) and is showing good agreement (~ 3 % variation) with simulated results as depicted in Fig.11. Deflection was found to increase from 2.8 nm to 44.5 nm with decrease in thickness from 0.5 µm to 0.2 µm, which shows the increased sensitivity of thinner beam. FEM results of deflection as a function of thickness for the first four shapes (shape-a; shape-b; shape-c, and shape-d) of cantilevers are shown in Fig.12.

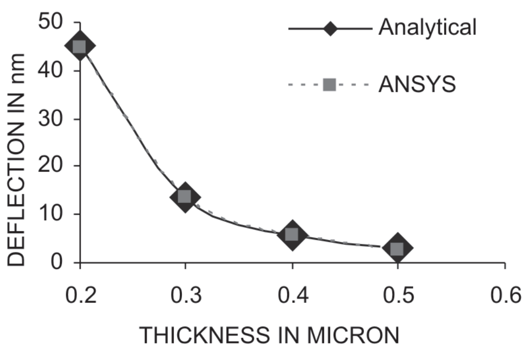

Figure 11. Deflection versus thickness calculated using analytical and FEM for rectangular shaped cantilever.

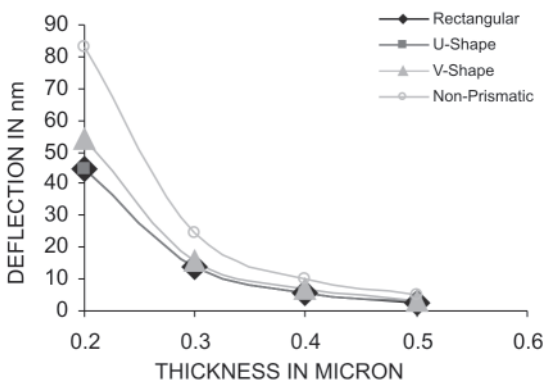

Figure 12. Deflection versus thickness of different shaped microcantilevers (shapes a to d).

It is clear from this graph that shape-b is giving the maximum deflection for the same thickness and is more suitable for sensor operation in static mode as compared to other structures. Deflection mapping of the various deformed cantilevers are shown in Figs 13 and 14 depicting deflection in µm at each point.

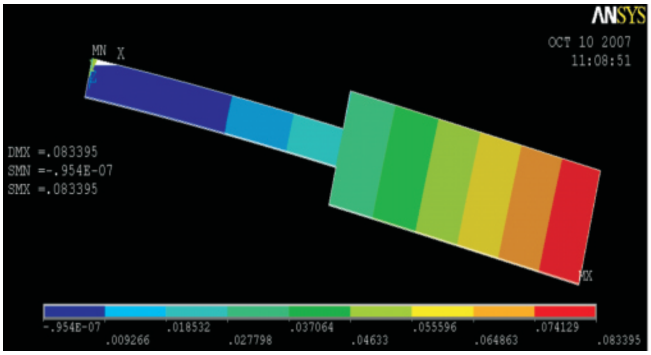

Figure 13. ANSYS output for deflection of microcantilever of shape-b.

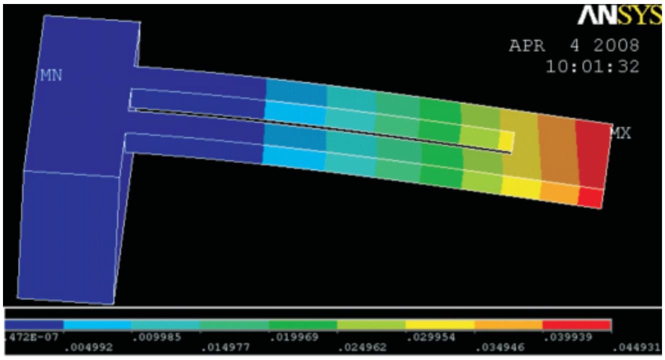

Figure 14. ANSYS output for the deflection of U-shaped microcantilever.

For operation in the dynamic mode, natural frequency of a rectangular shaped cantilever (shape-a) as a function of thickness was determined analytically as well as using ANSYS software. The results are plotted in Fig.15, showing good agreement (~ 4 per cent variation) between the two approaches.

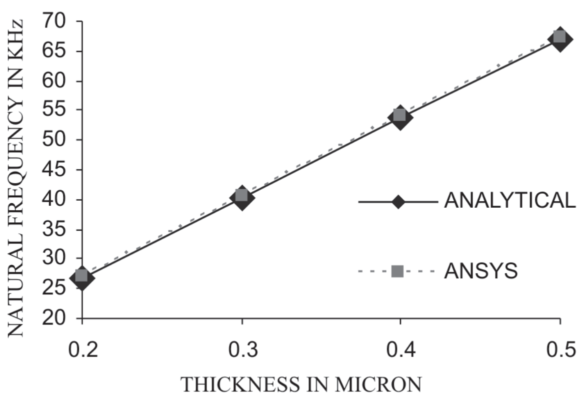

Figure 15. Natural frequency of rectangular cantilever calculated analytically and by ANSYS.

The resonant frequency was determined for all the six shapes keeping the length (100 µ) and thickness (0.5 µ) the same. The frequency shift due to attaching a small mass (~10-12 pg) on the upper side of the cantilever was calculated. Simulated results of dynamic mode are given in Table 1. It is clear from these calculations that conventional rectangular shape-a gives the smallest mass sensitivity whereas V-shaped geometry (shape-e) gives almost eight times more mass sensitivity than the conventional rectangular shaped microcantilever. But in case of V-shaped microcanilever, it is difficult to fabricate sharp tip at the end. So tapered V-shape (shape-f) has been considered for the analysis, which shows sensitivity more than four times as compared to conventional rectangular microcantilever.

Table 1. Natural frequency and mass sensitivity for different shaped cantilevers

Geometry of microcantilever	Natural frequency (KHz)	Mass sensitivity (Hz/pg)
Shape-a	67.74	43
Shape-b	40.19	52
Shape-c	59.12	86
Shape-d	98.94	186
Shape-e	117.49	344
Shape-f	99.89	228

Simulation regarding use of both sides of the cantilever has also been carried out and results show that sensitivity gets doubled by utilising both the surfaces of the microcantilever. So by utilising both the surfaces of the microcantilever in dynamic mode, one can increase the mass sensitivity.

In another set of FEA calculations, different materials were explored for the fabrication of microcantilevers. Presently researches are not limited to silicon as a material choice for the fabrication of these kind of sensors, but are being explored other materials such as silicon-oxide, silicon nitride and polymers like SU-8[16,17]. To see the effect of the material on sensitivity of these types of sensors, simulation was carried out for the tapered V-shaped (shape-f) cantilever. Properties of different materials like silicon, silicon oxide, silicon nitride and SU-8 have been used to get the sensitivity of the microcantilever in dynamic mode. Table 2 shows that the maximum mass sensitivity is obtained in case of SU-8 microcantilevers.

Table 2. Sensivity of various materials

Material	Sensitivity (Hz/pg)
Si	228
SiO_2	147
Si_3N_4	182
SU-8	302

6. CONCLUSIONS

- The simulation results of six different shapes have clearly shown that the sensitivity of the microcantilever-based sensors can be significantly improved by modifying the geometry and properties of the materials. V-shape is suggested for maximising the performance in case of resonant frequency shift mode and shape-b for maximising the deflection in static mode over the conventional rectangular-shaped microcantilever.

- Simulated results show that sensitivity is also dependent on the material properties like density and Young's modulus. For the shape-f, SU-8 microcantilevers show the maximum sensitivity. Therefore depending upon the application and detection procedure, suitable geometry and materials can be selected.
- Micromechanical platform offers an opportunity for the development and mass production of extremely sensitive, low-cost sensors for real-time *in situ* sensing of many chemical and biological species. Therefore, cantilever sensors with extremely high sensitivity can be fabricated by simply reducing and optimising the cantilever dimensions. However, decreasing the cantilever size results in increased difficulties in fabrication as well as monitoring of cantilever response. So by changing the geometry of the microcantilevers, one can increase the sensitivity of these types of sensors.

7. FUTURE PROSPECTIVES

The bending response of a single microcantilever is often influenced by various undesired effects, such as thermal drift and unspecific reactions taking place on uncoated cantilever surface resulting in additional cantilever bending. To avoid such kind of effects researchers have introduced microcatilever array. Sensor array offers several advantages over single sensor such as selectivity to a wide range of analyte, better selectivity, multiple component analysis etc. Figure 16 shows the FEA simulation of the array of six microcantilevers. Each microcantilever is in different loading conditions (10^{-2} μN to 3×10^{-2} μN) and showing different deflections accordingly.

In microcantilever array system, one cantilever is acted as reference cantilever, which will not react with the molecules of analyte. As difference in signal from the reference and sensor cantilever shows the net cantilever response, even low sensor response can be extracted from large cantilever deflection without being dominated by undesired effects. In the case of single microcantilver, no such kind of drift compensation is possible. By using an array of microcantilevers having different functionalised layer on each cantilever, researchers are developing 'Nose on a Chip' to sense various hazardous chemicals and explosives[18,19]. This technology holds the key to next generation of highly sensitive sensors and from the scientific point of view, the challenges lie in optimising cantilever sensors to improve their sensitivity to the ultimate limit, i.e., the detection of an individual molecule.

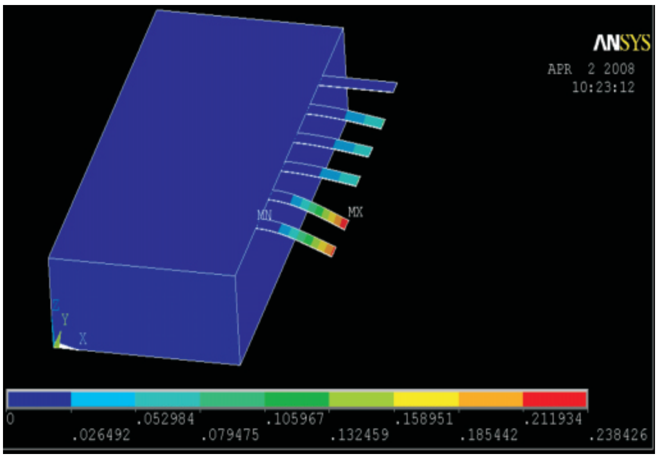

Figure 16. Deflection in microcantilever array.

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