Simulation of Biosensor using FEM

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Abstract: Bio-Micro Electro Mechanical Systems/Nano Electro Mechanical Systems include a wide variety of sensors, actuators, and complex micro/nano devices for biomedical applications. Recent advances in biosensors have shown that sensors based on bending of microfabricated cantilevers have potential advantages over earlier used detection methods. Thus, a simple cantilever beam can be used as a sensor for biomedical, chemical and environmental applications. Here, microfabricated multilayered cantilever beam is exposed to sensing environment. Lower layer being pure structural silicon or polymer and upper layer is of polymer with antigen/antibody immobilized in it. Obviously, it has an affinity towards its counterpart i.e. antibody/antigen. In the sensing environment, if counter elements exists, they get captured by this sensing beam head, and the cantilever beam deflects. This deflection can be sensed and the presence of counter elements in the environment can be predicted. In this work, a finite element model of a biosensor for sensing antibody/antigen reaction is developed and simulated using ANSYS/Multiphysics. The optimal dimensions of the microcantilever beam are selected based on permissible deflection range with the aid of MATLAB. In the model analysis, both weight and surface stress effects on the cantilever are considered. Approximate weights are taken into account because of counter elements, considering their molecular weight and possible number of elements required for sensing. The results obtained in terms of lateral deflection are presented.

Keywords: bio-MEMS, FEM modeling, poly-MEMS, bio-sensors.

1. Introduction
MEMS (Micro-Electro-Mechanical systems) are integration of micron sized sensors, actuators and associated electronics on a single substrate using microfabrication techniques. Microfabrication has entered every aspect of sensors. Micromachined biosensors are leading to small, portable, easy to use, low cost, fast, high performance and revolutionary handheld labs for chemical and biological analysis. Not only silicon but also some novel materials / biomaterials are being used in these systems. In most of these devices relative motion is an important factor. Bio-MEMS exploit a wide variety of physical and chemical transduction principles for both chemical sensing and measurement of bio-activities. Earlier MEMS were the results of exploiting the materials and processing techniques developed for integrated circuits(IC’s). In recent years, polymers have been extensively used as both structural and functional materials for micro-fabricated sensors. Nowadays, the area of development of MEMS on polymer substrate is gaining much importance. This is because of the advantages of polymers over silicon namely low cost, more flexibility, transparency to visible UV, easily mouldable capability,
Improved bio-compatibility and or bio-activity, possibility of making polymers with tailor-made properties by manipulating the very molecular structure.

Cantilever based sensors are based on relatively well known and simple transduction principle. “A simple cantilever beam can be used as a sensor for biomedical, chemical and environmental applications”. When microfabricated multilayered cantilever beam is exposed to sensing environment, it bends because of single or a combination of external forces like electrostatic, electric, magnetic, mass, nuclear radiation or mere mass. Similarly, it can bend because of intrinsic stresses generated due to chemical, physical or thermal means within the upper layer of cantilever itself. Current literature review on microcantilever sensors shows that the bending of microcantilever is mainly due to surface stresses generated. Immobilization of molecules on the cantilever surface is a prerequisite for the use of cantilevers as biosensors. The choice of molecule depends on the desired application in either liquid or gas phase. The molecules immobilized make the cantilever specifically sensitive to other molecules for which they have affinity. The molecular interaction on the cantilever surface makes the cantilever bend as a result of the surface stress induced by the interaction. Surface stress induced by molecular interactions is usually not observed on the surface of a bulk material. However, when the reaction occurs on the surface of a flexible cantilever, the surface stress strains the cantilever into bending. The cantilever is a stress sensor and bends in response to free energy changes on its surface.

Cantilever responses are assumed to be not mass-dependent and cantilever sensors therefore work equally well detecting both large and small molecules. It is difficult to give a physical interpretation of how biomolecules adsorption and biochemical reactions change surface stress. Microcantilever bending would involve models from very distinct scientific areas, such as molecular modeling, surface science, colloidal chemistry, and mechanical engineering. It is considered that bending is the result of combination of forces like mass, surface, interaction between the molecules, chemical changes and electrostatic forces. However, in this paper a mass sensitive cantilever is modeled, considering different dimensions and shapes.

Microfabricated multilayered cantilever beam is exposed to sensing environment. “Lower layer being pure structural polymer or silicon and upper layer as polymer with antigen-antibody immobilized in it”. Obviously, it has an affinity towards its counterpart i.e., antibody-antigen. In the sensing environment if there are counter elements, they will be captured by this sensing beam head, and cantilever beam becomes heavy and then deflects (Fig 1). This deflection can be sensed and the
presence of counter elements in the environment can be predicted. The same antigen-antibody reaction technique can also be used for enzyme-substrate reaction and ligand-receptor reactions and appropriate sensors can be built. Considering antibody (IgM) molecules distributed uniformly on the cantilever surface, and bending of cantilever is mainly due to weight of antigen (BSA), analysis is done. The idea here is to increase or intensify the density of antigens on the cantilever surface.

2. Theoretical model

The model considered is a uniform beam with a rectangular cross section, which is fixed at one end and free at the other. Range of dimensions for the cantilever beam are taken from earlier literature [1]. A multilayered cantilever beam of 100µm x 20 µm x 0.15 µm of silicon, and 100 µm x 20 µm x 0.02 µm of SU-8 is considered for the sensor (Fig.2a). Similarly, second model with same surface area but narrow at the fixed end (10 µm) and wide (30 µm) at the free end is also considered (Fig. 2b). Only weight as a factor of deformation is applied to this cantilever beam and deflection in terms of 1 to 10 nanometers were observed.

“Beams that are constructed of more than one material, can be treated by using an equivalent width technique. Here an equivalent cross section is developed considering the modulus of elasticity. For this equivalent cross section, centroid is located and moment of inertia along the centroidal axis is determined. Then the deflection is calculated. The following equations help in determining the equivalent moment of inertia of the equivalent beam (Fig 3).

The optimal dimensions of the microcantilever beam are selected based on permissible deflection range with the aid of MATLAB (Fig. 4a and 4b). Fig. 4a, shows graph of deflection sensitivity of the micro-cantilever with respect to length and thickness. Fig 4b shows graph of deflection sensitivity of the micro-cantilever with respect to URL and thickness.
\[
y = \frac{(A_1y_1 + A_2y_2)}{(A_1 + A_2)} = 0.07526 \text{ } \mu\text{m}
\]
\[
I_{xx} = \frac{b_1 (d_1^3)}{12} + b_1d_1(y_1^2) + \frac{b_2 (d_2^3)}{12} + b_2d_2(y_2^2) = 0.2459 \mu^4
\]

Modulus of elasticity of equivalent beam is taken same as that of SU-8

\[E = 4400 \mu\text{N}/\mu^2\]

Hence equivalent moment of inertia becomes

\[I_{eq} = 1081.96\mu\text{N}\times\mu^2\]

Deflection can be calculated by the following equation

\[\text{Deflection} = \frac{WL^4}{8EI_{eq}} = 1.30\text{nm}\]

3. Results and discussions

A cantilever of above said dimensions was modeled in ANSYS / Multiphysics and was subjected to different weights due to antigen molecules. The deflection of this sensor was done analytically and also with ANSYS / Multiphysics simulation. Both the results obtained were almost matching. “The problem is modeled using shell-91 element which is a quadrilateral element with 8-nodes⁴.” Shell-91 is used for layered applications of a structural shell model. This element has six-degrees of freedom at each node: translations in the nodal x, y and z directions and rotations about the nodal x, y and z axis. Following are the FEM results for model-1(Fig. 5) and model-2(Fig. 6). It is observed that the deflection is more for model-2 as the sensing head is wide and CG is near the tip. Thus model-2 is more sensitive though it has same sensing area.

**Fig. 4 a**  
**Fig. 4 b**

**Fig. 5 Deflection of Model 1**  
**Fig. 6 Deflection of Model 2**
The beam is modeled with the details as shown below

- **Silicon**: $E=1.9 \times 10^5 \, \mu N / \mu^2$ Layer thickness = 0.15$\mu$
- **SU-8**: $E=0.044 \times 10^5 \, \mu N / \mu^2$ Layer thickness = 0.02$\mu$

Similarly the same cantilever is subjected to differential surface stress between the range 0.008 N/m to 0.5 N/m. The results obtained are in the order of microns. “Cantilever bending is assumed according to Stoney’s equation and differential surface stress is proportional to change in Gibbs free energy caused by the adsorption process, mass of the bound analyte molecules per unit area and molar mass of the analyte”. The resulting deflections are shown in Fig. 8. A curve showing bending at the tip because of differential stress is shown in Fig. 9.

**4. Conclusion and future scope**

“Present work shows that, with sufficient number of antigen molecules adhering to antibody molecules coated on cantilever beam deflects only due to weight”. Similarly, when the same cantilever is subjected to differential surface stress between 0.008 n/m to 0.5 N/m, bending observed was in
microns. Comparing these values, one can say that bending is mainly because of surface stress changes and not because of weight. The results obtained by theoretical calculations for model-1 are agreeing with results obtained from ANSYS. Thus one can use ANSYS/Multiphysics for such small dimensions. MEMS are revolutionizing the development of biosensors. A simple cantilever beam or leaf spring can be used as a sensor for chemical, environmental and biomedical applications. These sensors will be small, portable, easy to use, low cost, disposable and highly versatile diagnostic instruments.

New materials, microstructures and transduction methods need to be explored further for use in biosensors, chemical and environmental sensors. MEMS based sensors should be integrated within tiny biochips with on-board electronics, sample handling techniques, and analyzing techniques.

Such theoretical results and their analysis will be of much interest to the people working on design and fabrication of microcantilever based sensors.

Acknowledgments
Authors are very much thankful to Prof. Rakesh Lal of IIT Bombay, Mumbai for his suggestions and timely help.

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