# Design Of Piezoelectric Microcantilever Chemical Sensors In COMSOL Multiphysics Area


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***Abstract-*** ***This paper offers an analytical modeling of thin-filmed, multi-layer piezoelectric microcantilevers that are used as MEMS sensors. These sensors are chemical kind and use piezoelectric microcantilever. These types of microcantilevers are covered with variety of unique probe coating. The sensor has high sensitivity with external voltage measured in mV and uses PSD[1] system to indentify chemical ingredients of materials. The identification of the chemical ingredient of materials is based on change in angle of micro cantilever in the liquid or gas environment. The deflection of microcantilever results in varying voltage that can be used to analyze materials. Analytical simulation using Cosmol software and theoretical computations using equations will be offered in order to determine the parameters for optimal design setting. The analytical simulation includes design of mems and Cosmol software model development. The analytical model of the cantilever will be analyzed and the process of its construction will be discussed.***



***Keywords— Piezoelectric 1, MEMS 2, Microcantilever 3,COMSOL modeling and simulation4 ,Chemical Sensors5.***


## I. Introduction

There have been significant advances in the area of thin-film, multi-layer piezoelectric with application to mems. These piezoelectric mems devices can be used in sensors and actuators. The chemical mems sensors function on the basis of the position sensitive sensors (PSD) as shown in "Fig. 1and 2".

This paper describes chemical sensors that function on the basis of piezoelectric principals to replace devices that function based on traditional PSD. The advantages of the new piezoelectric are high sensitivity, wide frequency response range, low electrical power consumption, high precision, and simplified instrumentation.

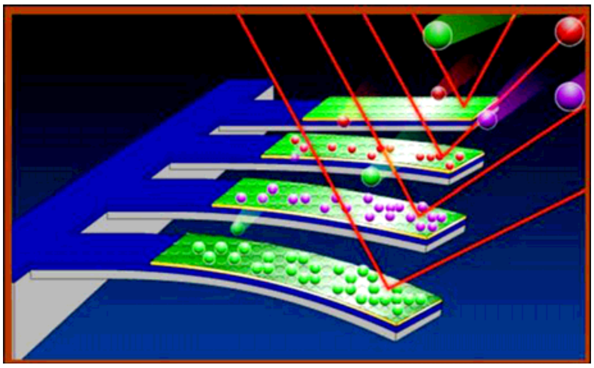


*Fig 1. scheme of PSD based sensor*

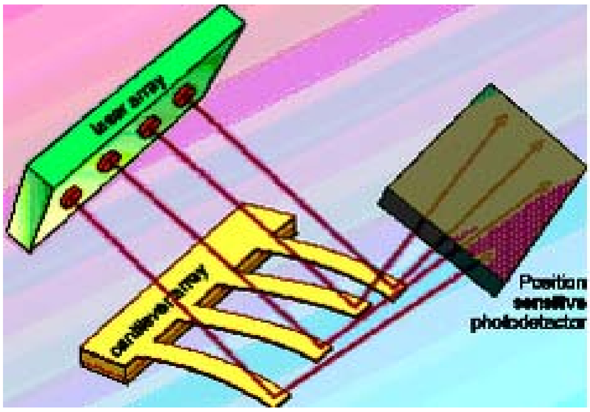



*Fig 2. scheme of Laser- based position detection system sensor.*

Lu1 et al offers the formula describing the mechanical properties of microcantilever piezoelectric[1,2]. Zhang et al developed the relationship between minimum measurable input force gradient and resulting deflection of piezoelectric microcantilever using scanning force microscopy[3,4]. Smits and Choi investigated electro- mechanical

[1] - Position Sensitive Sensors

characteristics of piezoelectric[5]. Cheng et al's study offers method of closed loop control to reduce effective error to measure deflection of multi-layer piezoelectric cantilever[6,7]. There is a need for analytical modeling and design of such piezoelectric based devices. The static and dynamic analytical modeling and simulation of micro cantilever piezoelectric is accomplished here by using Comsol software. In this paper, the mechanical and electrical properties of piezoelectric sensors will be determined using analytical simulation.

## II. Theoretical Considerations

In this paper, two methods are used to expose the process that determines electro mechanical parameters of multi-layer microcantilever. The first method uses mathematical formulation to analyze the relationship between applied surface contact pressure on the surface of the microcantilever and the resulting bending and displacement. Furthermore, the relationship between displacement and voltage is established. The second method is on the basis of analytical simulation of micro cantilever using Comsol software. The cantilever is composed of the following layers: Ti, Zno, Si3N4, Ti and SiO2 with the Ti located at the top of the cantilever and SiO2 is the bottom layer. In addition, a coating is applied to the surface of the cantilever. This sensor is used to analyze, measure, and expose the specific molecular and atomic structure of the liquid or gas being analyzed. These molecules and atoms are called target analyte. To attract analyte to the surface of the sensor, a special coating is applied to the surface of the sensor. Once there is a chemical reaction between analytes with the coating on the surface of the sensor, there is a chemical binding that result in some of the analytes to penetrate in between the probe coating atoms. This penetration results in surface pressure on the cantilever and thus cantilever deflection. Continuous measurement of amount of change in angle and voltage at piezoelectric layers allows exposing the chemical composition of the materials being analyzed. "Fig. 3" shows the side view of the designed cantilever with corresponding materials used in construction of it.

Once force is applied to the piezoelectric, the result is displacement of atoms in crystalline structure. This displacement of atoms results in varying electrical charge on the surface of the piezoelectric. The inverse of this process also results in displacement of the atoms. That is, once an external voltage is applied to the piezoelectric material, the atoms in crystalline structure displace due to change in center of electrical positive and negative charges which results in a net bipolar torque and a specific moment on the microcantilever. The direction of the moment applied to the microcantilever changes with reversal of the polarity. Once chemical reaction on the microcantilever occurs, the result is a differential surface stress that in turn results in cantilever deflection. This deflection can be written as

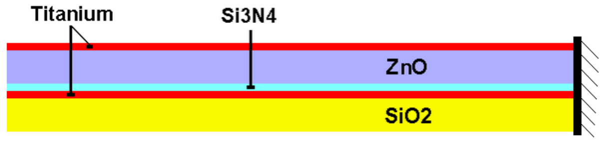



*Fig 3. Side view of the designed cantilever.*

$$Z = \frac{3(1-v)L^2}{T^2 E}\delta s \quad (1)$$

Where ν is Poisson ratio, L is cantilever length, δs is differential surface stress, T is cantilever thickness, and E is Young's modulus.

Let's assume that a thin layer of piezoelectric is placed on a thick elastic material. The elastic material is in static equilibrium and has no electrical charge. The relationship between deflection of the tip of cantilever and voltage is described using the following equation:

$$Z = d_{31}\frac{3L^2 Ep}{T^2 Ee}V \quad (2)$$

Solving for V in the above equation,

$$V = \frac{T^2 Ee}{3d_{31}L^2 Ep}Z \quad (3)$$

Where $d_{31}$ is the coefficient of piezoelectric material and $E_e$ and $E_p$ are the Young's moduli for elastic and piezoelectric material, respectively. Substituting equation (1) into equation (3) results in,

$$V = \frac{Ee(1-V)}{d_{31}E_p E}\delta s \quad (4)$$

The deflection of cantilever is in nanometer range and is based on amount of chemical reaction on the surface of the cantilever. Based on equation (1), for a microcantilever with dimensions 1.3, 17.5, and 70 micrometer and deflection of 2 nanometer, the computed regular differential surface stress is 0.24 N/m.

## III. Model description and analysis

The simulation modeling has been done using Comsol software since this software has the capability for design, modeling, and simulation of mems. For the purpose of simulation, the cantilever is constrained at one end and free at the other end. X direction is designated along the length of the cantilever. Furthermore, the followings conditions are applied:

1) Each layer of cantilever is in static equilibrium.

2) There is no shear displacement between layers of cantilever.

*TABLE 1. Description of cantilever layers.*

| Materials | Function | | | | | | |
|---|---|---|---|---|---|---|---|
| Titanium | Electrodes of piezoelectric layer | | | | | | |
| ZnO | Piezoelectric layer | | | | | | |
| Si3N4 | Used to insulate and cancel the initial charges in the cantilever | | | | | | |
| SiO2 | Flexible basic layer of the cantilever | | | | | | |
| **Structure** | **Length** | **Width** | **thickness** | **Titanium** | **ZnO** | **Si3N4** | **SiO2** |
| Unit (μm) | 70 | 17.5 | 1.3 | 0.1 | 0.5 | 0.1 | 0.5 |

3) All layers are in form of solid rectangular shape with equal length, L, and width, W. However, the thickness of the layers varies.

4) The total pressure is applied in XY plane and the average surface pressure is represented by δs. The meshed model has the following dimension: 70 μm × 17.5 μm (l × w) and 1.3 μm in thickness. There are 70000 to 80000 elements in the model. The meshed model of the micro cantilever is shown in“ Fig. 4”.
Once analytes make chemical reaction with the surface of the sensor, the resultant is a surface pressure on the surface of the sensor.

In this paper, a small pressure is applied such that the molecules can exert force on the surface of the sensor in vertical Z direction. The resulting voltage generated by piezoelectric is measured. This measured voltage and other information are used to determine the real behavior of the piezoelectric.

## IV. Results and discussions

The model for multi layer piezoelectric cantilever is based on solid three dimensional elements. The length, width, and thickness of the cantilever are 70, 17.5, and 1.3 micrometer, respectively. The ratio of length to width for this simulation is 4:1. The selected layer of piezoelectric is Zno. Due to relative large value for coefficient of piezoelectric, Ti is selected as the electrode due to its low Young modulus value. The force applied by the molecules on the surface of the piezoelectric is in Z direction. The deflection due to applied force is between 60 to 830 nanometers. The result of simulation reveals that generated voltage decreases with increase in length (Fig. 5).

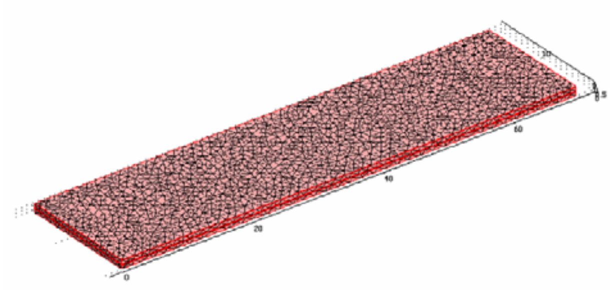
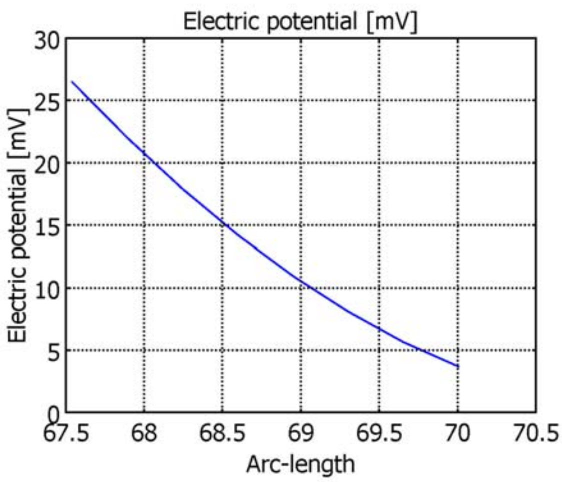


*Fig4. meshed model of the designed micro cantileve .*




*Fige 5. Generated voltage versus microcantilever length.*

Based on equation (3), voltage and length have inverse relationship. $(T/L)^2$ describes the straight line relationship between deflection and length of cantilever.

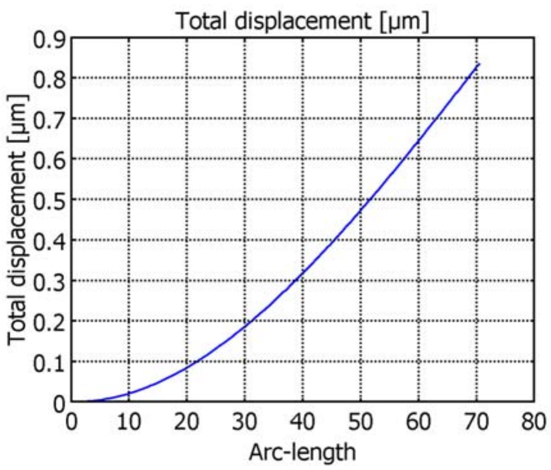



*Fig 6. The relation between microcantilever length and corresponding displacement in it (as the result of specific load).*

If the load is applied on the surface of the cantilever for duration of one second, the deflection increases linearly with increase in load application time (Fig. 7).

There is a negligible difference between the results based on analytical simulation and the results generated using equations described in this paper. This difference is due to lower and upper electrodes where the dimensional values of their Young's modulus are not accounted for in the computations. The maximum external voltage achieved from the recommended type of such a sensor with a piezoelectric thickness of 0.5 µm is 4 to 26 mV. Thick layers of piezoelectric results in a greater voltage generation. This is not a recommended practice due to reduced sensor sensitivity and increase in cost and complexity.

## V. proposed fabrication process

The fabrication process starts with a silicon wafer and a thin layer of $SiO_2$( Fig *8*) . The following steps are proposed to be completed in order to fabricate piezoelectric mems microcantilever:

With the wafer and a thin layer of $SiO_2$, using standard lithography process, form the primary layer of cantilever structure. This would allow the pattern of microcantilever beam to be transferred to one side of the layer. Next, a thin layer of Ti is laid. This layer acts the bottom electrode contact. To isolate the $SiO_2$ layer from the piezoelectric layer, $Si_3N_4$ is laid in this step. Zno films should be laid next. Using RF sputtering, the Zno film pattern on the surface of the microcantilever is developed. Thermal annealing at 460ºC is performed in this step in order to reduce the compressive residual stress of ZnO layer described in step 4 of this process. Sputtering Ti on the structure to act as the top electrode is the next step of this

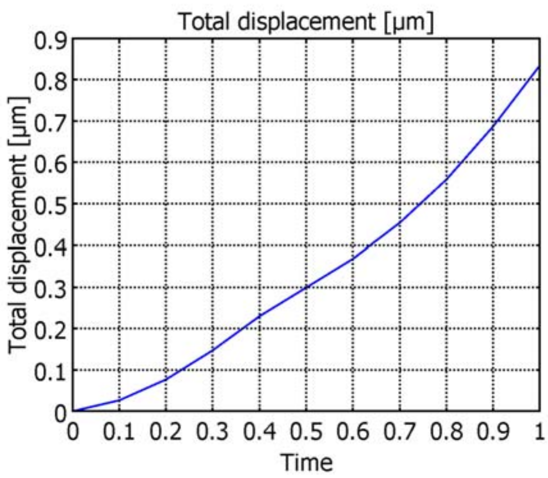



*Fig 7. Total displacement versus applying load time duration.*

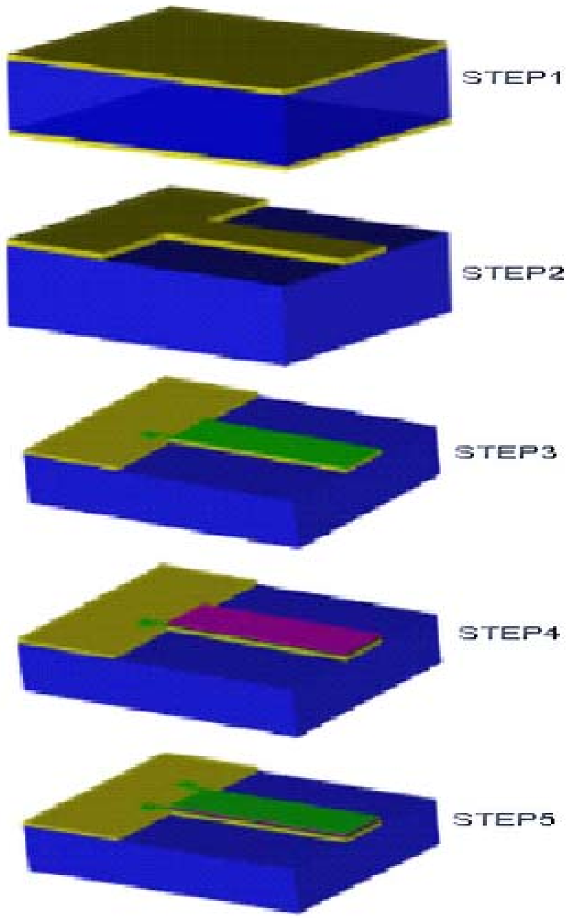



*Fig 8. Fabrication steps for piezoelectric microcantilever chemical sensor.*

process. As the final step, in order to form the microcantilever structure, photoresist mask is applied.

## VI. Conclusion

Using Comsol software to design and simulate a five layer micro cantilever, its mechanical and electrical properties were determined. An analytical model is developed for the thin-film multi-layer microcantilever chemical sensor. Analytical simulation of mechanical and piezoelectric of such sensor has been completed and the results generated correlates with results based on equations referenced in this paper. The microcantilever studied in this paper is one of the smallest micro cantilevers that should lead to development of microcantilevers measured in nanometer scale. The piezoelectric sensor was designed such that the voltage generated is on scale of mV. The voltage generated for a sensor of length 70 µm is in the range of 4 to 26 mV. This range of voltage is suitable for sensing electronic systems. Increase in thickness of piezoelectric layer results in increase in generated voltage. However, this increased voltage is not desirable due to sensor sensitivity reduction and increase in cost and loss. This research improves the design and performance of piezoelectric sensors by specifying the primary design parameters for optimal sensor functionality.

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