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Development of a Novel Design and Modelling of MEMS Piezoelectric Cantilevers-Based Chemical Sensors †

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Abstract: Analytical modelling of thin-film, multilayered piezoelectric microcantilevers is presented in this work. Piezoelectric microcantilevers are used in these chemical sensors. Different types of probe coatings are applied to these types of microcantilevers. A Position-Sensitive Sensor (PSS) system is used to identify chemical ingredients in the materials with high sensitivity, and external voltage is measured in mV. The maximum voltage generated for the sensor is 39 mV. This range of voltage is suitable for sensing electronic systems. An angle change of a microcantilever in a liquid or gas environment identifies a material's chemical ingredients. A microcantilever deflects, resulting in varying voltages to analyze materials. COMSOL software and equations will be used for analytical simulations to determine optimal design parameters. COMSOL software model development and MEMS design are involved in analytical simulations. This paper examines the analytical model of the cantilever and discusses the fabrication process.

Keywords: MEMS; piezoelectric; MEMS; microcantilever; COMSOL modelling and simulation; chemical sensors

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1. Introduction

Thin-film, multilayer piezoelectric has made significant advances with applications to MEMS. A piezoelectric MEMS device can perform both sensor and actuator functions. Piezoelectric sensors are highly sensitive, have a broad frequency response range, require little power, are highly precise, and simplify instrumentation.

MEMS cantilevers with sensitivity and Aluminium Nitride (AlN) as piezoelectric material have been exploited [1,2]. The mechanical properties of the piezoelectric microcantilever described with the formula have been reported [3,4]. An analysis of the relationship between the minimum measurable input force gradient and the deflection of piezoelectric microcantilevers was conducted using scan force microscopy [5,6]. A study of the electromechanical characteristics of piezoelectric has been conducted [7]. Researchers suggest a closed-loop control method to measure the deflection of multilayer piezoelectric cantilevers [8,9]. Micro cantilevers coated with antibodies (blue-green) that capture viruses (red spheres). As the cantilevers identify and capture more virus molecules, one or more of the mechanical or electrical characteristics of the cantilevers can change and be detected by an electronic interface. The size of the particle being detected and captured is one of the factors affecting the size of the cantilever. These antibodies are proteins produced in the blood in response to the presence of an antigen (e.g., virus, bacteria, toxin). Devices based on piezoelectric need to be modelled and designed analytically. COMSOL software is used here to model and simulate micro cantilever piezoelectric statically and dynamically. In this paper, piezoelectric sensors are described, and their mechanical and electrical properties are determined through analytical simulations.

2. Sensor Design and Modelling

A multilayer microcantilever is examined in this paper using two methods for determining its electromechanical parameters. First, a mathematical formulation is employed to investigate the relationship between surface pressure applied on the microcantilever surface and its bending and displacement. Also, the displacement-voltage relationship is established. Second, microcantilever simulations are performed using the COMSOL software. The cantilever is composed of Molybdenum (Mo) as top and bottom electrodes, and the piezoelectric layer of Aluminium nitride (AlN) is embedded between them.

Furthermore, the cantilever surface is coated. The sensor analyses, measures, and exposes liquids and gases' molecular structure and atomic composition. Target analytes are molecules and atoms that are used as measurements. Sensor surfaces are coated with special coatings to attract analytes. When analytes and the coating on the sensor's surface react chemically, a chemical binding results in some analytes penetrating between the atoms of the probe coating. Cantilever deflection results from surface pressure on the cantilever caused by this penetration. Piezoelectric layers can be continuously measured to reveal their chemical composition by measuring the angle and voltage. The side view and materials used to construct the designed cantilever are shown in Figure 2.

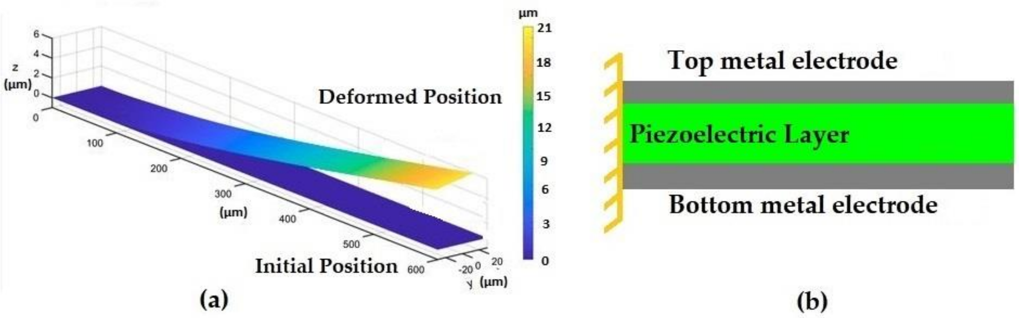

Figure 2. (**a**) Microcantilever simulated in the deformed position. (**b**) A side view of a microcantilever that was designed.

Piezoelectric devices cause atoms in crystalline structures to move when force is applied. Due to this displacement of atoms on the piezoelectric surface, the electrical charge varies. Inversely, this process also results in atom displacement. When the polarity is reversed, the moment applied to the microcantilever changes direction. Deflection of the microcantilever happens when a chemical reaction occurs on its surface. The deflection can be expressed as follows:

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

where v is the Poisson ratio, L is length, δs is differential surface stress, T is the thickness, and E is Young's Modulus.

Assume that a thin piezoelectric layer is placed over a thick elastic material. There is no electricity in the elastic material because it is in static equilibrium. The relationship between the deflection of a cantilever's tip and voltage can be expressed as follows.

$$Z = d_{31}\frac{3L^2 E_p}{T^2 E_e}V \tag{2}$$

In the above equation, find V.

$$V = \frac{T^2 E_e}{3d_{31} L^2 E_p} Z \tag{3}$$

Assume that d_{31} represents the coefficient piezoelectric material and E_e and E_p represent the elastic piezoelectric material's Young's modulus. Substituting Equation (1) into Equation (3) results in.

$$V = \frac{E_e \left(1 - V\right)}{d_{31} E_p E} \delta s \tag{4}$$

3. Simulation Setup and Parameters

COMSOL software is used for simulation modelling because it can model, simulate, and design MEMS. When the simulation is performed on a cantilever, one end is constrained while the other is free. Cantilevers are designated along their length in the X direction. Additionally, the following conditions applied; There is a static equilibrium between every cantilever layer. Between layers of the cantilever, there is no shear displacement. Each layer consists of a solid rectangular shape with equal length (L) and width (W). However, each layer differs in thickness. It is assumed in the model that an average surface pressure δs is applied to it, and that the pressure is distributed in the XY plane. Surface pressure is created on the sensor surface when analytes react with its surface. Molecular force is exerted on the sensor's surface in a vertical Z direction under a slight pressure applied here. It measures the resultant voltage generated by piezoelectric devices. Piezoelectric behaviour is determined based on this voltage measurement and other information. Non-linearities in MEMS (Micro-Electro-Mechanical Systems) cantilever beams is essential for improving their performance and reliability. It can arise from various sources, including material properties, geometry, and operating conditions. The specific approach will depend on the nature of the non-linearities, the application, and the available resources. Here are some approaches to address non-linearities in MEMS cantilever beams like Design Optimization, Material Selection, Pre-Stress Control, Operational Parameters, Feedback Control, Modeling and Simulation, Sensing Techniques, Calibration and Compensation, Advanced Control Strategies, Experimental Validation.

Table 1. MEMS Cantilever layer description with properties.

Material	*Thickness*	*Poisson Ratio*	*Density [g/cm³]*	*Young Modulus [GPa]*	*Relative Permittivity*
Molybdenum	*200 nm (Top-Bottom)*	*0.29*	*10.1*	*315*	*1*
Aluminum Nitride	*1.5 μm*	*0.27*	*3.30*	*348*	*9*

4. Results and Discussion

Piezoelectric cantilevers are constructed from solid three-dimensional elements. These microcantilevers have a length of 100–600 μm, a width of 50 μm, and a thickness of 1.9 μm, respectively. Molecules on the piezoelectric surface apply force in the Z direction. Due to the applied force, there is a deflection between 6 μm and 21 μm. Increasing length decreases generated voltage, according to simulation results. The maximum electric potential was achieved at 39 mV with a 600 μm cantilever length, as shown in Figure 3.

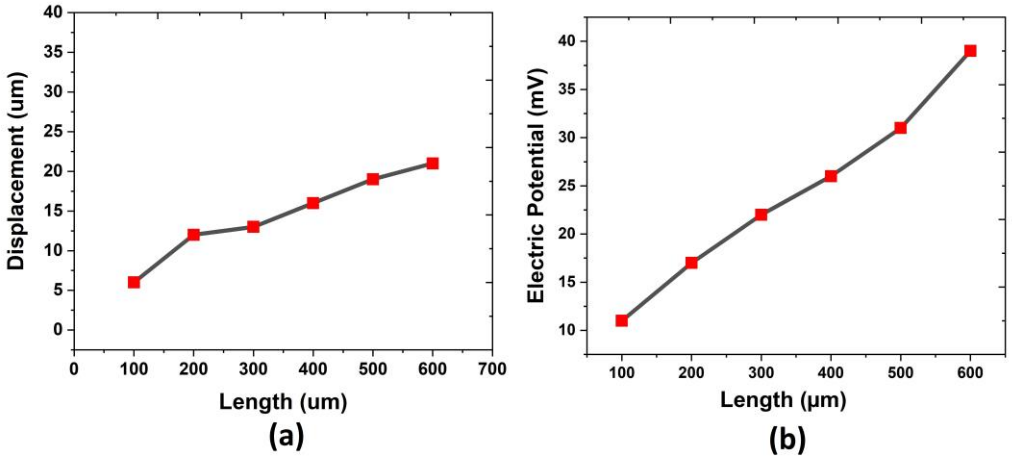

Figure 3. (**a**) Microcantilevers displacement vs. length (**b**) Microcantilever Electric potential vs. length.

The piezoelectric sensor was designed such that the voltage generated is on scale of mV. The voltages generated for the micro cantilever were in the range of 11 to 39 mV. This range of voltage is suitable for sensing electronic systems. Increase in thickness of piezoelectric layer results in increase in generated voltage. This research improves the design and performance of piezoelectric sensors by specifying the primary design parameters for optimal sensor functionality.

5. Proposed Microfabrication Process

The materials used for sensor fabrication are described with their properties, including the thin piezoelectric material layers in Section 3. The fabrication process will consist of different steps, including patterning the bottom metal electrodes (Figure 4a). The piezoelectric layer and the top electrode are patterned in the second step, as shown in Figure 4b. The MEMS cantilever is released from the substrate (Figure 4c). For releasing the cantilever, ICP etching of silicon with SF6 at very low temperatures and at very low pressures was used to produce isotropic etch profiles of silicon as shown in Figure, which help the cantilever to be released from the substrate. 700 sscm of SF6, coil power of 2600 W and pressure of 100 mTorr at temperature 18C° were applied for silicon etching. Figure 4 shows the entire flow process predicted for the fabrication of MEMS cantilevers.

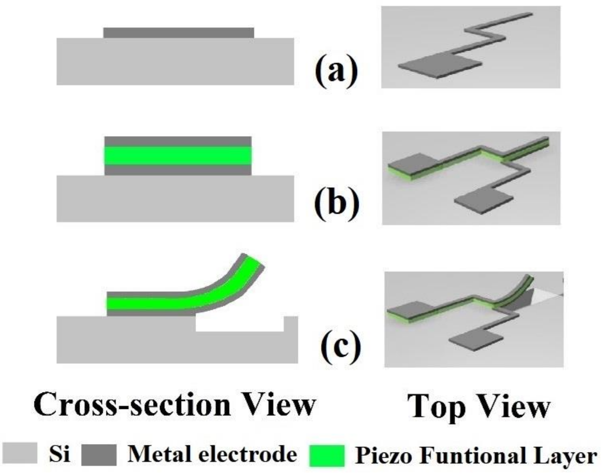

Figure 4. Fabrication steps for piezoelectric microcantilever chemical sensor. (**a**) Bottom electrode patterning. (**b**) Top electrode patterning together piezoelectric layer (**c**) Release of the cantilever from Si substrate.

A chemical MEMS sensor works with a Position Sensing System (PSS) shown in Figure 5.

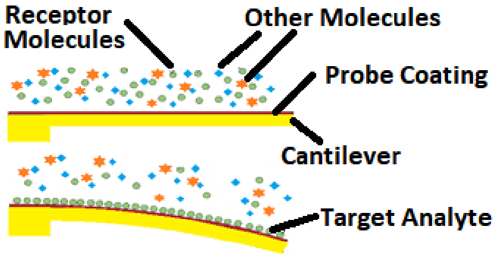

Figure 5. MEMS cantilever bending induced by molecular adsorption.

6. Conclusions

The mechanical and electrical properties of the microcantilever were determined using COMSOL software. Microcantilever chemical sensors based on thin-film multilayers are analyzed analytically. A mathematical simulation of such sensors' mechanical and piezoelectric characteristics has been completed, and the results generated correlate with those obtained using the equations provided in this paper. As a result of the piezoelectric sensor's design, voltage is generated on the mV scale. The maximum voltage generated by a sensor of length 600 µm with a displacement of 21 m is 39 mV. The voltage range obtained can be used to detect electronic systems. The voltage generated by piezoelectric layers increases with thickness. On the other hand, increased voltage decreases sensor sensitivity and increases costs and losses. This research enhances piezoelectric sensor performance by specifying primary design parameters.

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