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Development of a Novel Design and Modeling of MEMS Piezoelectric Cantilever-Based Chemical Sensors †

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

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

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1. Introduction

Thin-film, multilayered piezoelectric technology has made significant advances in application in 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 high sensitivity and aluminum nitride (AlN) as the piezoelectric material have been exploited [1,2]. The mechanical properties of the piezoelectric microcantilever described with the appropriate formula have been reported [3,4]. An analysis of the relationship between the minimum measurable input force gradient and the deflection of the piezoelectric microcantilevers was conducted using scan force microscopy [5,6]. A study of the electromechanical characteristics of piezoelectric sensors has been conducted [7]. Researchers suggest a closed-loop control method to measure the deflection of multilayered piezoelectric cantilevers [8,9]. Microcantilevers are 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 through 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, or toxin). Devices based on piezoelectric technology need to be modeled and designed analytically. COMSOL software was used here to model and simulate a microcantilever piezoelectric sensor 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 Modeling

A multilayered microcantilever was examined in this work using two methods for determining its electromechanical parameters. First, a mathematical formulation was employed to investigate the relationship between the surface pressure applied on the microcantilever's surface and its bending and displacement. Also, the displacement–voltage relationship was established. Second, microcantilever simulations were performed using COMSOL software. The cantilever was composed of molybdenum (Mo) as the top and bottom electrodes, and a piezoelectric layer of aluminum nitride (AlN) was embedded between them.

Then, the cantilever surface was coated. The sensor analyzes, 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 1.

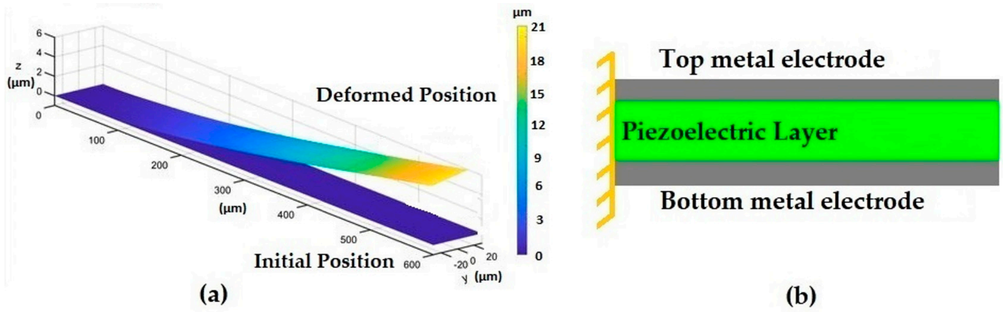

Figure 1. (**a**) Microcantilever simulated in the deformed position. (**b**) A side view of a microcantilever that was designed.

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. The deflection of the microcantilever happens when a chemical reaction occurs on its surface. The deflection can be expressed as follows:

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

where v is the Poisson ratio, L is the length, δs is the 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.

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

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

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

3. Simulation Setup and Parameters

COMSOL software is used for simulation modeling because it can model, simulate, and design MEMS. When the simulation was performed on a cantilever, one end was constrained while the other was free. Cantilevers were designated along their length in the X direction. Additionally, the following conditions were applied: There was a static equilibrium between every cantilever layer. Between layers of the cantilever, there was no shear displacement. Each layer consisted of a solid rectangular shape with equal length (L) and width (W). However, each layer differed in thickness. It was assumed in the model that an average surface pressure δs was applied to it, and that the pressure was distributed in the XY plane. Surface pressure was created on the sensor surface when analytes reacted with its surface. Molecular force was exerted on the sensor′s surface in a vertical Z direction under the slight pressure applied here. It measured the resultant voltage generated by the piezoelectric devices. Piezoelectric behavior was determined based on this voltage measurement and other information. Nonlinearities in the MEMS (micro-electromechanical systems) cantilever beams are essential for improving their performance and reliability. They can arise from various sources, including material properties, geometry, and operating conditions. The specific approach depends on the nature of the nonlinearities, their application, and the available resources. Here are some approaches to address nonlinearities in MEMS cantilever beams: design optimization, material selection, prestress control, operational parameters, feedback control, modeling and simulation, sensing techniques, calibration and compensation, advanced control strategies, and experimental validation. Table 1 shows the materials properties of the MEMS cantilever.

Table 1. MEMS cantilever layer descriptions with properties.

Material	Thickness	Poisson Ratio	Density [g/cm^3]	Young's 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 were constructed from solid three-dimensional elements. These microcantilevers had a length of 100–600 µm, a width of 50 µm, and a thickness of 1.9 µm, respectively. Molecules on the piezoelectric surface applied force in the Z direction. Due to the applied force, there was a deflection between 6 µm and 21 µm. Increasing the length decreased the generated voltage, according to the simulation results. The maximum electric potential was achieved at 39 mV with a 600 µm cantilever length, as shown in Figure 2.

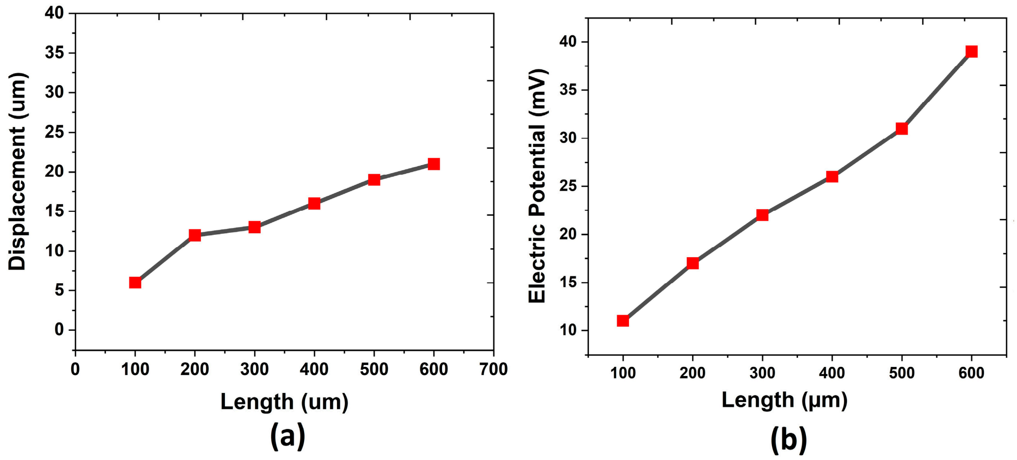

Figure 2. (**a**) Microcantilevers' displacement vs. length. (**b**) Microcantilevers' electric potential vs. length.

The piezoelectric sensor was designed such that the voltage generated was on the scale of mV. The voltages generated for the microcantilever were in the range of 11 to 39 mV. This range of voltages is suitable for sensing electronic systems. An increase in the thickness of the piezoelectric layer resulted in an increase in the 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 consisted of different steps, including patterning the bottom metal electrodes (Figure 3a). The piezoelectric layer and the top electrode were patterned in the second step, as shown in Figure 3b. The MEMS cantilever was released from the substrate (Figure 3c). For releasing the cantilever, an 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 the figure, which help the cantilever be released from the substrate. In total, 700 sscm of SF6, a coil power of 2600 W, a and pressure of 100 mTorr at a temperature of 18 °C were applied for the silicon etching. Figure 3 shows the entire flow process predicted for the fabrication of the MEMS cantilevers.

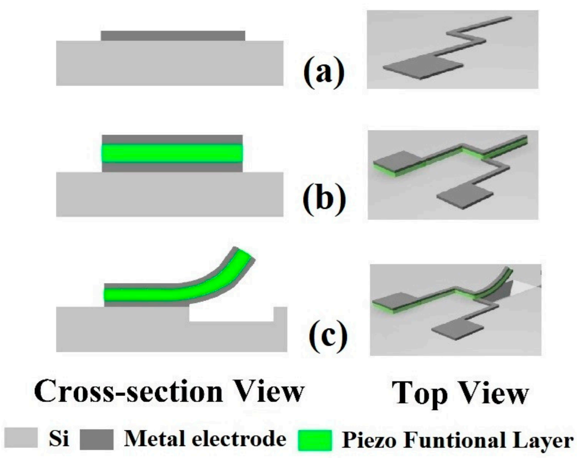

Figure 3. Fabrication steps for piezoelectric microcantilever chemical sensor. (**a**) Bottom electrode patterning. (**b**) Top electrode patterning for the piezoelectric layer. (**c**) Release of the cantilever from the Si substrate.

A chemical MEMS sensor works with a position sensing system (PSS), as shown in Figure 4.

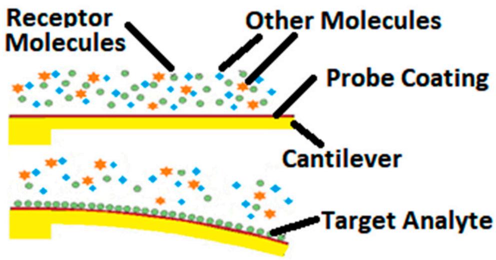

Figure 4. MEMS cantilever bending induced by molecular adsorption.

6. Conclusions

The mechanical and electrical properties of a microcantilever were determined using COMSOL software. Microcantilever chemical sensors based on thin-film multilayers were analyzed analytically. A mathematical simulation of such sensors' mechanical and piezoelectric characteristics was 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 was generated on the mV scale. The maximum voltage generated by a sensor of length 600 µm with a displacement of 21 m was 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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