Parametric Study of Polyimide – Lead Zirconate Titanate Thin Film Cantilivers for Transducer Applications

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Abstract: This paper reports the simulation of the piezoelectric actuation of micro-cantilevers. Lead Zirconate Titanate (PZT) was chosen for the device fabrication design, due to its thin film processing flexibility. Four layers compose the cantilever structures presented in this work: PZT (piezoelectric material), Platinum (electrodes) and Zirconium Oxide as the buffer layer for the PZT film and polyimide as the structural elastic material. COMSOL Multiphysics® was used in order to simulate the d33 mode and calculate the appropriate configuration parameters of the interdigitated electrodes to obtain larger cantilever deflections. A comparison of the d31 and d33 is also presented simulating both: two and three-dimensional models.

Keywords: PZT, Piezoelectric effect, bimorph actuator, cantilever beam.

1. Introduction

Micro-Electro-Mechanical Systems (MEMS) technology is based in microelectronics fabrication methods. The wide variety of materials available in this technology delivers advantages such as miniaturization and multiple components on a single chip for integrated Microsystems. These mentioned systems could be more consistent, less expensive, smarter and also less invasive than traditional macroscopic components and systems that could potentially be replaced.

In this paper we investigate the deflection of micro cantilevers using the piezoelectric actuation mechanism. The piezoelectric effect is a reversible process, which exhibits the so-called direct effect (internal generation of electrical charges resulting from an applied mechanical force) and its reverse effect (internal generation of a mechanical strain when an electrical field is applied).

Due to its versatility of thin-film processing, Lead Zirconate Titanate (PZT) was chosen for the design of this project. PZT is the most common piezoelectric ceramic in use today, which exhibits a high coupling coefficient. Both sputtering and sol-gel have been researched for MEMS as well as other electronic technologies for more than 30 years [1].

2. Theory

Typically piezoelectric actuators are designed as a cantilever beam or membrane. These consist of a thin structural material that supports the whole structure with a ferroelectric film between a top and a bottom electrode, as shown in Fig. 1 a). This makes use of the d31 piezoelectric coefficient (transverse strain constant). The in-plane strain X1 in the piezoelectric film is induced by an external electric field E3 normal to the plane. When a voltage is applied to the electrodes, the piezoelectric film contracts laterally for E3 parallel to the remnant polarization (Pr) of the film, which makes the beam bend up.

An interdigitated electrode can be used for a larger electric field and polarization in plane with the ferroelectric film, as shown in Figure 1 b). The induced strain X3 results from an in plane electrical field E3. This transverse piezoelectric strain bends the cantilever; this mode in use is the d33 mode (extensional strain constant). The d33 coefficient is approximately twice the d31 coefficient; therefore the expected deflection actuated by the d33 coefficient is larger [1].

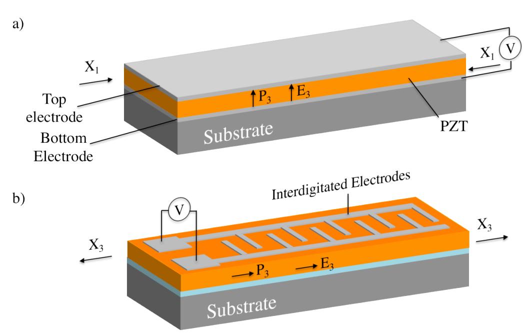

Figure 1. A schematic diagram of a cantilever actuated by a) d31 mode and b) d33 mode.

2.1 Piezoelectric Constitutive Equations

Basically the interaction between mechanics and electrical fields of a structure is called piezoelectricity. This interaction is modeled as the coupling of linear elasticity equations and electrostatic charge equations using electric constants. Piezoelectricity has been mathematically described using a material's constitutive equations [2-10]. These equations define how the Strain (S), Stress (T), Electric field (E) and the charge density displacement (D) interact between them [2]. The relation between the latter can be expressed in the stress-charge constitutive form:

$$T = c_E S - e^T E$$
$$D = eS + \varepsilon_T E$$

Or in the strain-charge constitutive form:

$$S = s_E T + d^T E$$
$$D = dT + \varepsilon_T E$$

The stress-charge form is usually used in finite element method due to the useful match to the PDEs of Gauss' law (electric charge) and Navier's equation (mechanical stress) [3].

Usually most material's data is given in the strain-charge form, which can be transformed into the stress-charge form by the conversion equations shown below:

$$c_E = s_E^{-1}$$
$$e = ds_E^{-1}$$
$$\varepsilon_S = \varepsilon_0 \varepsilon_{rT} - ds_E^{-1} d^T$$

3. COMSOL Multiphysics setup

The Piezoelectric Devices module was used for both two and three-dimensional simulations. A parameterized geometry was created in order to alter the structure geometry in a simple manner, by only modifying the values of the parameter's table. Predefined materials were added to the model from the material browser. Four different materials compose the cantilevers stack: polyimide (structural material), platinum (electrical material), lead zirconate titanate "PZT-5H" (piezoelectric material) and zirconium dioxide "ZrO2" (buffer layer). The PZT-5H properties are listed below using the strain-charge form:

Compliance matrix (ordering: xx, yy, zz, yz, xz, xy):

$$S_E = \begin{bmatrix} 16.5 & -4.78 & -8.45 & 0 & 0 & 0 \\ -4.78 & 16.5 & -8.45 & 0 & 0 & 0 \\ -8.45 & -8.45 & 20.7 & 0 & 0 & 0 \\ 0 & 0 & 0 & 43.5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 43.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 42.6 \end{bmatrix} * 10^{-12} \frac{m^2}{N}$$

Coupling matrix (ordering: xx, yy, zz, yz, xz, xy):

$$d = \begin{bmatrix} 0 & 0 & 0 & 0 & 741 & 0 \\ 0 & 0 & 0 & 741 & 0 & 0 \\ -274 & -274 & 593 & 0 & 0 & 0 \end{bmatrix} * 10^{-12} \frac{C}{N}$$

Relative permitivy :

$$S_E = \begin{bmatrix} 3130 & 0 & 0 \\ 0 & 3130 & 0 \\ 0 & 0 & 3400 \end{bmatrix}$$

The matrix components of the PZT-5H properties have a default poling direction in the z-axis. A local coordinate system (rotated 90 degrees about the global y-axis) was used in the material settings to rotate the piezoelectric material.

3.1 Design parameters

The parameters used for this project were selected based on the available materials and tools for fabrication of the micro devices in the NanoFab facilities at King Abdullah University of Science and Technology. Table 1 shows a list of the initial chosen parameters used for both 2D and 3D simulations. These parameters are only for the simulation of the d33 mode (extensional strain coefficient).

The d31 mode (transverse strain coefficient) was simulated to compare the deflection against the initial d33 actuated cantilever parameters. The d31 mode cantilever is a stack of a PZT-5H (0.5µm thick) sandwiched between two platinum plates [30µm (width)*120µm (length)* (0.3µm thick)], as shown previously in Figure 1.

Table 1: Initial d33 mode cantilever parameters.

Parameters	
Electrodes width	3 [µm]
Electrodes length	15 [µm]
Gap	3 [µm]
Cantilever length	120 [µm]
Cantilever width*	30 [um]
PZT thickness	0.5 [µm]
ZrO2 thickness	0.1 [µm]
Polyimide thickness	1 [µm]
Platinum thickness	0.3[µm]

*Only for 3D model

The geometry of the interdigitated electrodes used for the extensional coefficient mode actuation is shown in Figure 2. The schematic shows the parameters of the geometry that were used in the parametric sweep to change the model features.

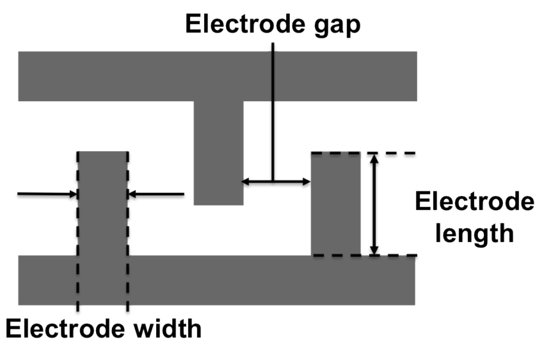

Figure 2. Parameterized interdigitated electrodes geometry.

A cross-section view of the d31 and d33 configuration for the actuation of the cantilever is shown in Figure 3.

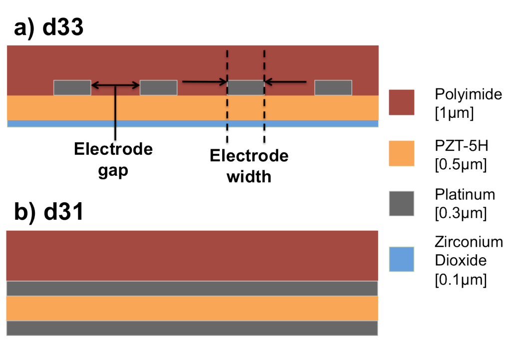

Figure 3. Cross-section view of a) d33 and b) d31 cantilever configurations.

4. Results

For the first simulation we could see a significant difference between d31 and d33 mode, see Figure 4. A total tip displacement of the d31 mode of 0.1102µm using 10 volts in comparison to the lowest displacement given by the two dimensional d33 mode configuration (gap = 15µm, electrode width = 1µm) of 0.2048µm at the same electric potential and physics setup. From these results it can be see that d33 mode generates a larger deflection of the cantilever.

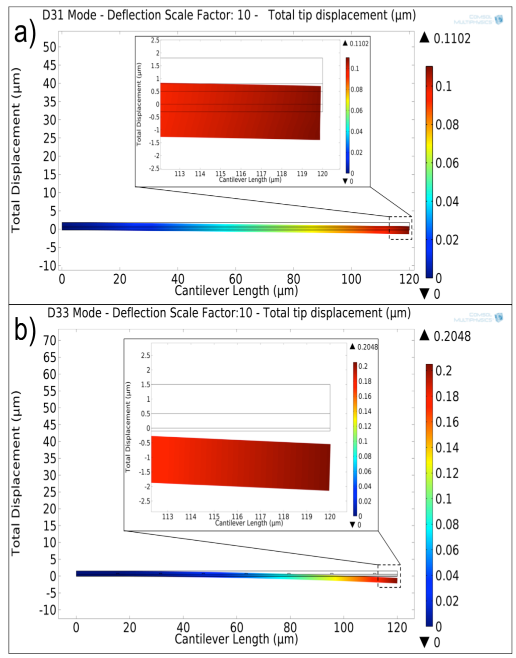

Figure 4. Comparison of a) d31 mode deflection and b) d33 mode deflection.

The largest deflection obtained from the 2D simulation was 2.427µm and 2.35µm from the 3D simulation. The differences between the 2D and the 3D simulations are due to features that are present in the 3D model but not possible in the 2D model. Features such as: carrier width and extra structural material that is not under the interdigitated electrodes area.

A variation of the electrodes width and gap parameters was performed using a parametric sweep in the COMSOL study configuration. The parametric sweep was done to determine the optimal configuration of the studied parameters.

The cantilever length was set to 120µm for all the simulations, the electrodes width and gap was evaluated ranging from 1µm to 15µm with a step of 2µm, getting 8 data points for each parameter. The actuation voltage was set to 10 Volts. The results of the 2D and 3D simulations are shown in Figure 5 and 6 respectively.

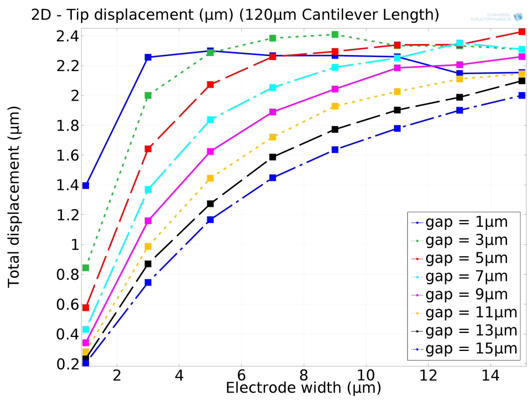

Figure 5. 2D simulation - Tip displacement parametric study. Parameters changing: gap and finger width.

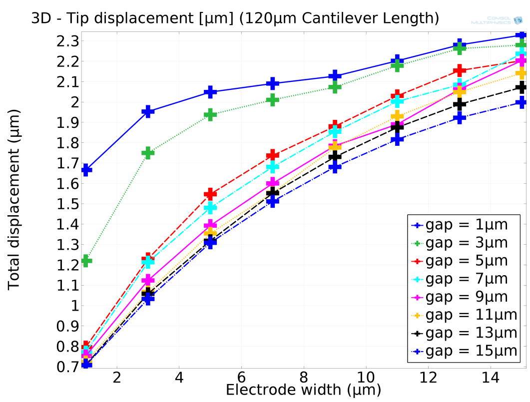

Figure 6. 3D simulation - Tip displacement parametric study. Parameters changing: gap and finger width.

From both graphs above, it can be seen that there is a limit (asymptote) at approximately 2.5µm of the total displacement, where the inverse piezoelectric effect starts to show a strange behavior in respect to the cantilever's deflection. This means that the design of the d33 mode should not use that configuration zone, to avoid any discrepancy in the cantilever's working range.

In both 2D and 3D simulations the trend is noticeable. It can be observed from Figure 5 and 6, that using larger electrodes width actually increases the final cantilever deflection until it reaches its working limits. In contrast, with a larger gap between the electrodes the cantilever's deflection is decreased.

5. Conclusions

A parametric simulation study was conducted to find optimal values for the cantilever configurations. Important physical parameters of the cantilever structures were varied in two-dimensional and three-dimensional models. The extensional coefficient (d33) actuation mode gave the largest deflection for the stack of materials used for the cantilever structure.

The studied structures are currently under fabrication and the experimental measurements will be compared against the numerical models. The fabrication designs are cantilever arrays with a combination of the following parameters: gap (3, 5 and 7µm), electrode width (3 and 5µm) and four cantilever lengths (120, 200, 275 and 350µm). Furthermore, studies regarding the material thicknesses and cantilever lengths will be performed.

The direct piezoelectric effect can also be used for sensing applications (i.e. accelerometers, flow sensors, energy harvesters). The initial results of the presented work are intended to understand the working principle of the presented cantilevers for the development of more complex micro devices.

6. References

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