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DESIGN, MODELING AND OPTIMIZATION OF A MULTILAYER THIN-FILM PZT DIAPHRAGM USED IN PRESSURE SENSOR

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Abstract

Multilayer thin-film PZT diaphragm has been designed and modeled. Commercial Finite element software, ANSYS was implemented to model the diaphragm. This multi-layer diaphragm can be used as both sensor and actuator. A simplified model is introduced to reduce the CPU time. Dynamic characteristics of the multilayer diaphragm have been investigated. The important parameters of the multilayer PZT diaphragm have been optimized to improve the performance of a pressure sensor using APDL macro. Some simple relation was found which can be used to predict the PZT layer characteristics in larger model with more elements.

Keywords: Finite Element, ANSYS®, MEMS Pressure Sensors, Multilayer Thin Film PZT Diaphragm, Piezoelectric

1. Introduction

During recent years, the study of micro electromechanical system (MEMS) has shown significant opportunities for micro sensors and microactuators based on various physical mechanisms such as piezoresistive, capacitive, piezoelectric, magnetic, and electrostatic. Piezoelectric MEMS offer many advantages compared to other MEMS technologies [1]. Many works have been done on the MEMS pressure sensors since 1970's [2]. Ravariu et al. modeled a pressure sensor designed to compute blood pressure. They use of the ANSYS simulation in order to estimate the mechanical stress in the structure [3]. Zinck et al. presented the fabrication and characterization of silicon membranes actuated by thin piezoelectric films [4]. Liu et al. designed two novel piezoelectric microcantilevers with two piezoelectric elements (bimorph or two segments of PZT films) and three electric electrodes [1]. The finite element method is a technique in which a given domain is represented as a collection of simple domains, called finite elements, so that it is possible to systematically construct the approximation functions needed in a variation or weighted-residual approximation of the solution of a problem over each element. We considered the structure shown in Fig.1 for the sensor.
In present work, design, modeling and optimization of a PZT membrane which is used in a pressure sensor is done by implementing ANSYS® finite element (FE) software.
In previous works only the membrane has been considered in simulation and the track of top electrode and its configuration were neglected. In this work the membrane is modeled completely. The simulation results can be used to study the characteristics and structural behaviors of this type of pressure sensor. Important parameters are optimized to obtain better response in a pressure sensor. Using this result huge amount of CPU time can be saved in modeling larger models with more elements.

2. Design and modeling of the PZT layer

Using the constitutive relations for a plate, equation of motion and charge can be written as:

$$c_{ijkl}u_{k,lj} + e_{kij} j_{,kj} + r f_i = r\ddot{u}_i \tag{1}$$

$$e_{ikl}u_{k,li} - e_{ij} j_{,ij} = r_e \tag{2}$$

Where *u* is the mechanical displacement vector, j is the electric potential, r is the known reference mass density, r_e is the body free charge density, *f* is the body force per unit mass. The coefficients c_{ijkl}, e_{kij} and e_{ij} are the elastic, piezoelectric and dielectric constants. The designed structure of the multilayer thin-film PZT diaphragm is shown in Fig. 1. The PZT layer cross section is schematically illustrated in Fig. 2. In this Figure ***a*** expresses the width of square multilayered diaphragm, ***d*** is the total width of the sensor which is approximately equal to 3***a***, and h_7 is thickness of the substrate. h_1, h_2 … h_6 are the thickness of each layer. The PZT layer was deposited on Pt/Ti/SiO_2/Si wafer via sol-gel process. Au layer was evaporated on the surface of PZT film as the top electrode. The backside silicon was wet etched off till the SiO_2 layer [6].
Since the substrate is made of anisotropic wet etched Si(100) wafer, the etched angle is known of around 54.7°. Therefore, the dimension of *c* can easily be determined by following equation:

$$c = \frac{1}{2}(d - a) - h_1 \cot(54.7^o) \tag{3}$$

The materials properties of each layer within the diaphragm which is in the FE modeling are listed in Table 1. There is E is Young's modulus (GPa); μ is Poisson ratio; ρ is density ($\times 10^3$kg/m^3) and h is thickness (μm).

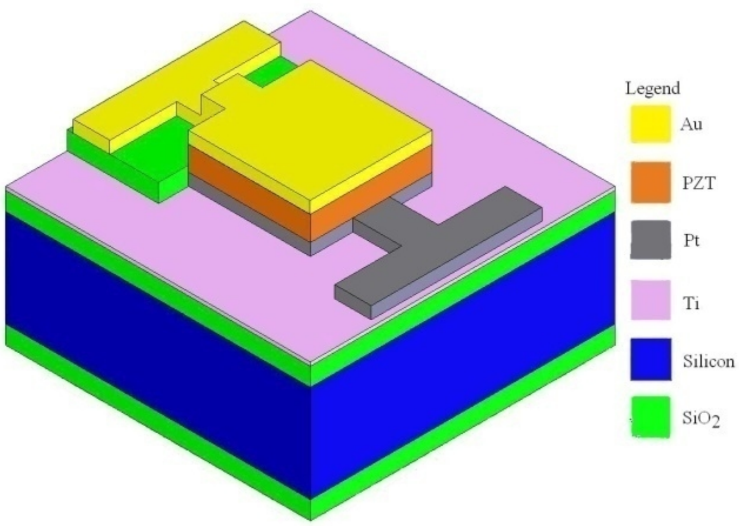

Fig. 1. Structure of the multilayer PZT diaphragm

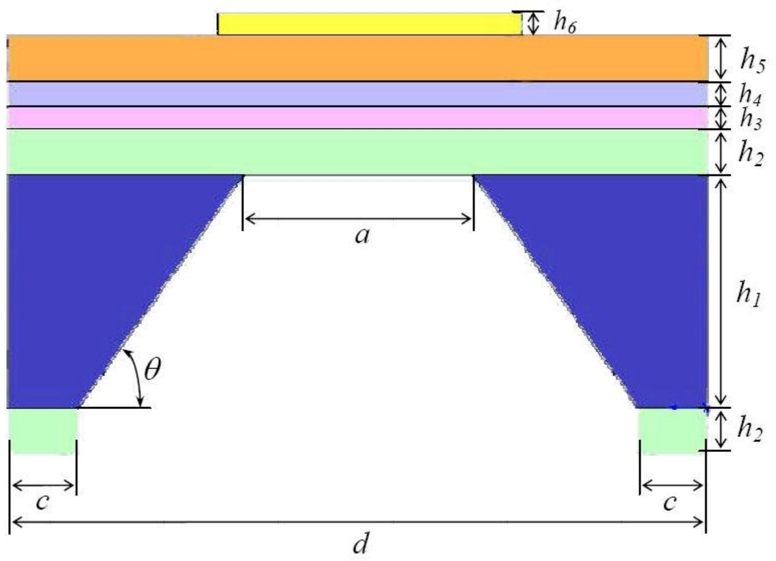

Fig. 2. Cross section of the structure of the diaphragm

Table 1. The properties of each material in the structure

Layer	Material	Thickness	E	µ	ρ
h_1	Si	500 μm	190	0.33	2.33
h_2	SiO_2	400 nm	72.4	0.16	2.07
h_3	Ti	25 nm	102.1	0.3	4.85
h_4	Pt	200 nm	146.9	0.39	21.45
h_5	PZT	1 μm	86.2	0.287	7.62
h_6	Au	200 nm	80	0.42	19.32

3. Finite Element Modeling

The micro piezoelectric sensor was modeled in ANSYS FE software to obtain its electro-mechanical characteristics.

Three different element types were adopted to characterize different layers in the device. Solid 46 element type which has the capability of modeling the layered solid was used to model elastic layers of Pt, Ti and SiO_2. Using this element type helped modeling of three solid layers in one element layer. Piezoelectric layer was modeled using Solid5 element type. Substrate and Au layers were modeled using solid 45 element type.

The small thickness-width ratio is the most challenging issue in the FE modeling of the thin films. Huge amount of elements are required to achieve suitable aspect ratio. In the present work, three layers of elements in modeling the membrane and substrate requires huge amount of CPU time. Some author used simplified model to decrease the CPU time [6], only modeled the diaphragm and substituted the surrounding membrane and substrate effect with clamped boundary condition. This simplified model is very rigid boundary condition. In this study a simplified model was used which assume that the substrate is a rigid body. The nodes in the interface between substrate and membrane were fixed. Modeling the thin film layers offers more relaxed boundary condition than one which is used in [6] despite its need to more CPU time.

Half model was used in simulation due to the symmetry of the structure and to reduce modeling time and hardware requirement, as it's shown in Fig. 3.

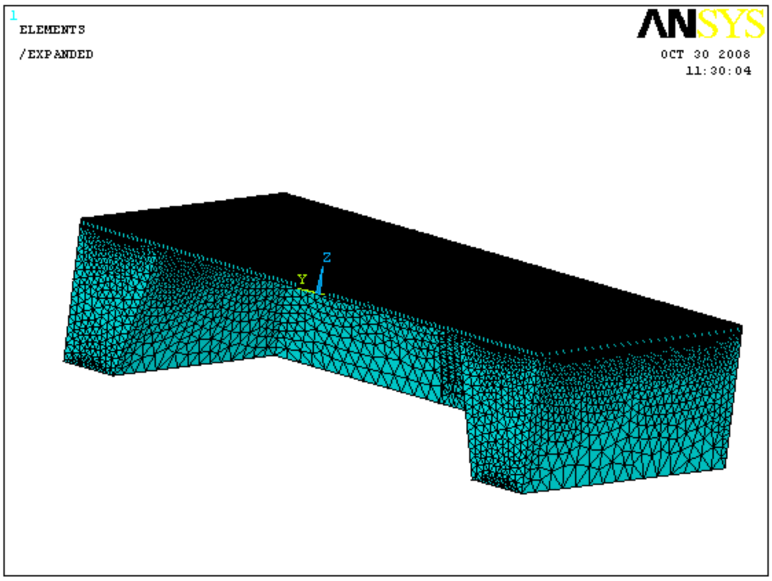

Fig. 3. The model used in ANSYS®

3.1. Validation of numerical analysis

The accuracy of the finite element method results depends on element type, model discretization, and solution controls which are used in the analysis. Thus the model and solution controls should be evaluated before using the FE model in the further analysis. The numerical, analytical results of frequencies of two-layered clamped PZT plate [7] were used to verify our numerical analysis process by using ABAQUS FE-codes. As mentioned in [8] the clamped square plate was laminated by an elastic layer of SiO_2 and a PZT layer of $PbZr_{0.54}Ti_{0.46}O_3$ with $1\mu m$ in thickness, respectively. Table 2 compares the five natural frequencies obtained by ANSYS FEM software and by theoretic calculation and ABAQUS FEM software at different width of the square plate. The errors, based on ANSYS data, are within 1.30% as comparing with the results in [7] is shown in Fig. 4. This comparison indicates the acceptance of the analysis method and element sizes used in the ANSYS FEM software.

Table 2. Comparison of the first five nature frequencies for a clamped square $PbZr_{0.54}Ti_{0.46}O_3/SiO_2$ laminated plate with each Layer of Thickness at 1 μm*.

		Width						
		100 μm	200 μm	300 μm	400 μm	500 μm	750 μm	1000 μm
Model 1	ANSYS	1378.74	344.59	153.13	86.11	55.09	24.47	13.73
	ABAQUS	1364.31 (1.05%)	342.352 (0.65%)	152.262 (0.57%)	85.669 (0.51%)	54.834 (0.46%)	24.373 (0.40%)	13.711 (0.14%)
	Theory	1388.747 (0.73%)	347.1868 (0.75%)	154.3052 (0.77%)	86.7967 (0.80%)	55.5499 (0.83%)	24.6888 (0.89%)	13.8875 (1.15%)
Model 2,3	ANSYS	2810.4	702.3	311.96	175.4	112.23	49.84	28.02
	ABAQUS	2773.57 (1.31%)	697.892 (0.63%)	310.55 (0.45%)	174.758 (0.37%)	111.867 (0.32%)	49.728 (0.22%)	27.974 (0.16%)
	Theory	2831.78 (0.76%)	707.945 (0.80%)	314.6422 (0.86%)	176.9863 (0.90%)	113.2712 (0.93%)	50.3428 (1.01%)	28.3178 (1.06%)
Model 4	ANSYS	4136.11	1034.12	459.4	258.41	165.33	73.37	41.261
	ABAQUS	4074.16 (1.50%)	1027.7 (0.62%)	457.526 (0.41%)	257.511 (0.35%)	164.852 (0.29%)	73.287 (0.11%)	41.228 (0.08%)
	Theory	4175.461 (0.95%)	1043.865 (0.94%)	463.9401 (0.99%)	260.9663 (0.99%)	167.0184 (1.02%)	74.2304 (1.17%)	41.7546 (1.20%)
Model 5	ANSYS	5029	1256.8	558.6	313.84	200.75	89.06	50.09
	ABAQUS	4953.65 (1.50%	1251.29 (0.44%)	557.209 (0.25%)	313.644 (0.06%)	200.796 (0.02%)	89.27 (0.24%)	50.22 (0.26%)
	Theory	5073.002 (0.87%)	1268.251 (0.91%)	563.6669 (0.91%)	317.0626 (1.03%)	202.9201 (1.08%)	90.1867 (1.27%)	50.73 (1.28%)

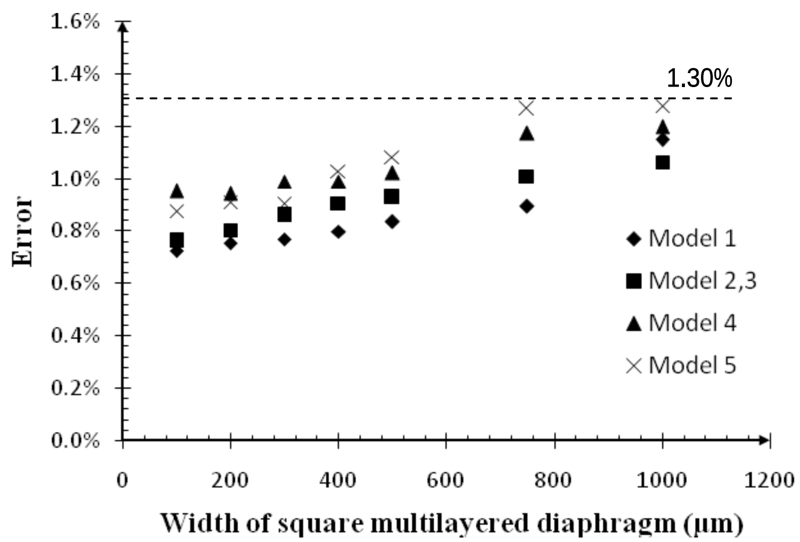

Fig. 4. The errors, based on ANSYS results based on Table 2

3.2. Effect of substrate and track of Au

Some errors were happened in the simplified model due to assuming the substrate as a rigid body. To investigate on the effect of this simplification, static and modal analyses were performed on the simplified and exact model. The 1^{st} and 5^{st} natural frequency errors in two models as comparing with exact model are compared in the Table 3. There is small error between two models and the simplified model can be used in the further static and harmonic analyses.

Table 3. Effect of substrate and track of Au on nature frequencies

Nature Frequencies (kHz)		Exact model	Simplified model with Au track	Simplified model without Au track
Mode	1^{st}	415	420 (1.21%)	408 (1.68%)
	5^{st}	1542	1560 (1.16%)	1520 (1.42%)

* The percent ratios in brackets are the frequency errors between exact model and simplified model with Au track and without Au track.

4. FE Results and Optimization

The effect of important parameters on the behavior of the exact model is investigated in this section. Fig. 5 shows the displacement, stress in different directions, total stress, and strain at 40 mbar pressure. The dimensions of the model of a multilayer diaphragm that is used for obtain this results were a = 300 μm and h_5 = 1 μm. As shown in Fig. 5 the maximum displacement of the diaphragm is at the center, and the maximum stresses in different direction are along the edges of the diaphragm.

4.1.Effect of dimension of diaphragm on the natural frequency

Fig. 6 show the influence of the width of the square multilayer PZT diaphragm on the first nature frequency. The natural frequency decreases rapidly with increasing the diaphragm width especially in the larger PZT layer thicknesses. The x-axis of Fig. 6 was replaced with the reciprocal area of diaphragm, $1/a^2$, and is shown in the Fig. 7. As can be seen there is a linear relation between the 1^{st} natural frequency and reciprocal area of diaphragm. Fig. 8 shows the 1^{st} natural frequency versus PZT layer thickness in the different diaphragm widths. There is also a linear relation between the 1^{st} natural frequency and PZT layer thickness. Fig. 7 and 8 can be used to predict the natural frequency in the larger models with more elements without further simulation. The dimension of the real MEMS sensors are larger than the sensor modeled in present work. There is three layers in the model, modeling a sensor which its dimension is 2 times larger than this model, require 12 times more elements than this model. Solving this huge amount of elements requires huge amount of CPU time to solve and hardware to save the model data.

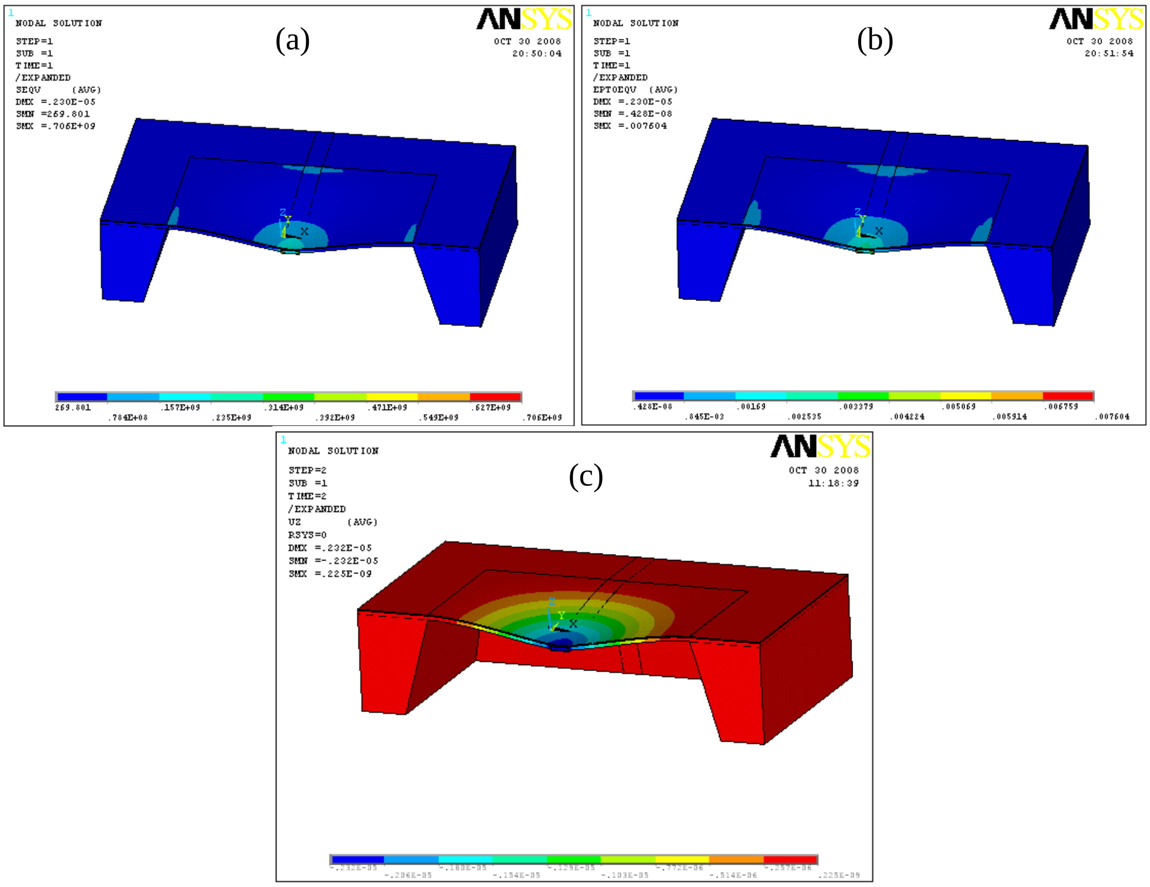

Fig. 5. The simulation result from ANSYS (a) Stress total; (b) strain; (c) displacement

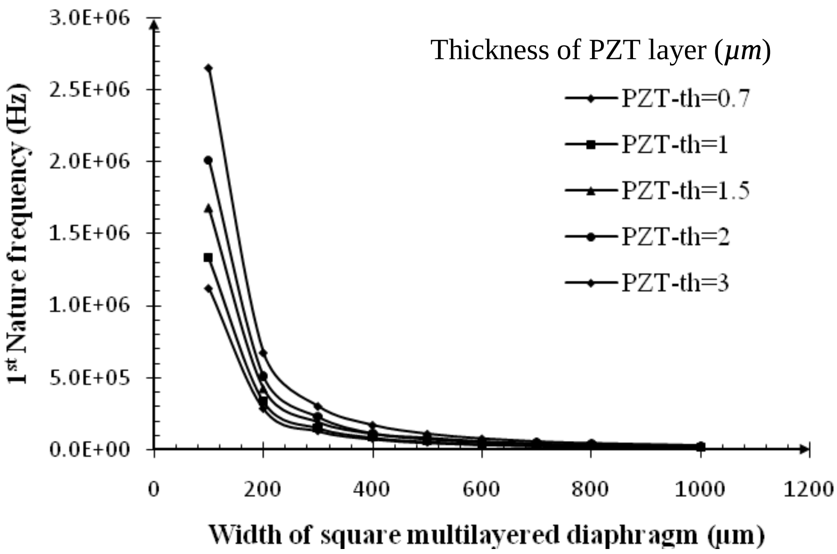

Fig. 6. Change of the first nature frequency of structure via the variation of width of square laminated diaphragm

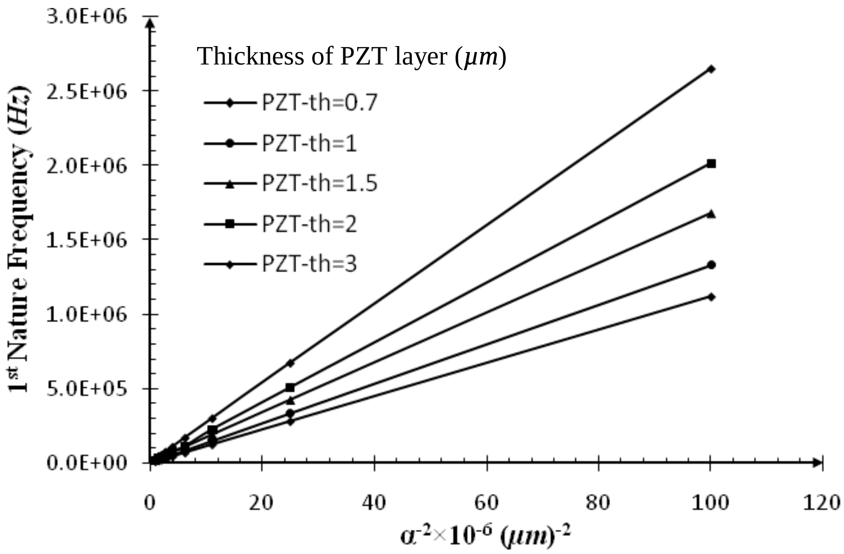

Fig. 7. Change of the first nature frequency of structure via the inverse of square of width, $1/a^2$, of square laminated diaphragm

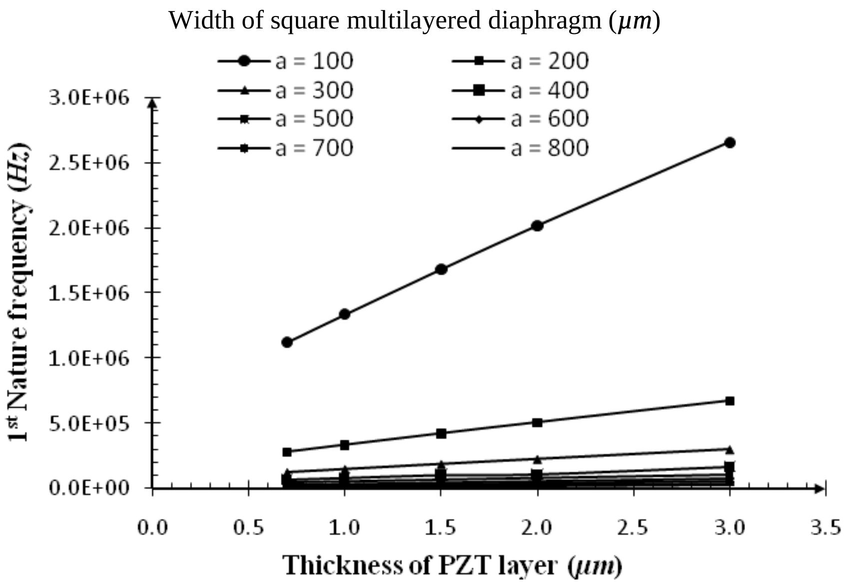

Fig. 8. Effect of thickness of PZT-layer on the structure nature frequency

4.2. Harmonic response of the PZT thin film diaphragm

Harmonic response of the sensor was investigated under applying pressure load on the diaphragm. A damping ratio equal to 0.015 was assumed in the analysis. Fig.9 shows the deflection response at center point of the diaphragm. The voltage response PZT layer is shown in the Fig.10. The dimensions of the exact model of a multilayer diaphragm which is modeled were a = 250μm, d = 750μm, h_1 = 200μm and h_5= 1μm.

There is a little difference between the exact model and adopted simple model result and can be neglected. The exact model took CPU time 2.15 times more than simple model. As is shown in section 3.2, Table 3, the simple model can be used in further harmonic analysis in order to save the CPU time and reduce analysis cost.

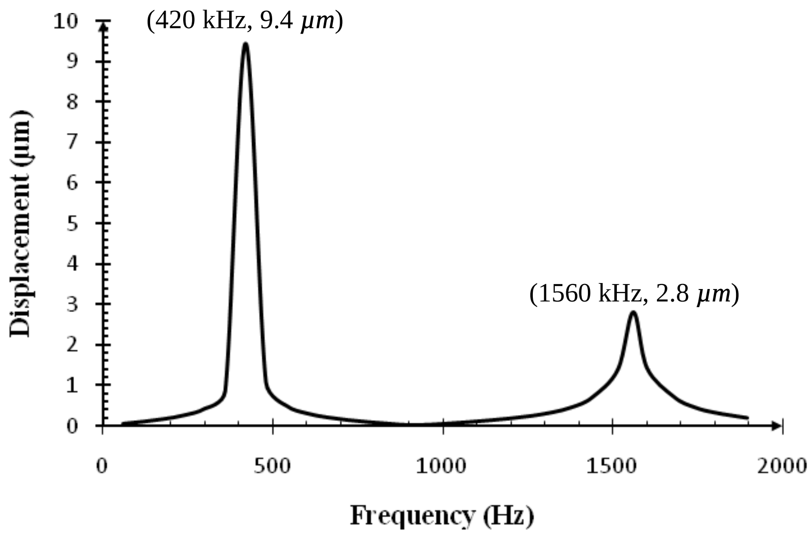

Fig. 9. Displacement at centre point of the diaphragm

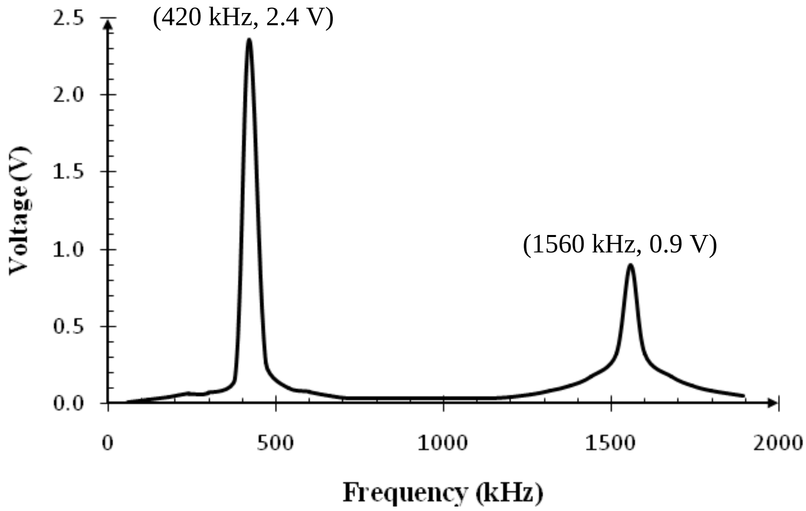

Fig.10. voltage response in PZT-layer at centre point of the diaphragm

4.3. Effect of thickness ratio on dynamical behavior of the PZT thin film diaphragm

The deflection of the diaphragm depends on various parameters. The effect of some of these parameters on the dynamic response of sensor was investigated in previous sections. Optimization processes should be done to select a suitable set of parameters which yield to good response. The ratio of PZT layer Thickness to other layers thicknesses are examples of this important parameters and should be optimized. In this study the effect of PZT layer thickness ratio to SiO_2 layer, named "R", on the deflection of center point is investigated. For a constant SiO_2 layer thickness, if the thickness of the PZT layer tends to zero or infinity there will no actuation under applying constant voltage. Thus there is an optimum R which the center point of diaphragm has the maximum value. The effect of R on the center point of the membrane in various diaphragm widths is shown in Fig.11. The R ratio was changed using different SiO_2 layer thickness and the PZT layer thickness remained constant at h_2 =

$1\mu m$. As can be seen in each diaphragm width there is an optimum thickness ratio. The optimum value of R depends on the PZT layer thickness too. An optimization code was written in the ANSYS Parametric Language Design (APDL) to obtain the optimum value of R in different diaphragm widths and PZT layer thicknesses. Fig.12 shows the optimization results obtained from the written macro. These curves can be used to predict the optimum value of R in larger models with more elements and save many CPU time and hardware required to save the model data.

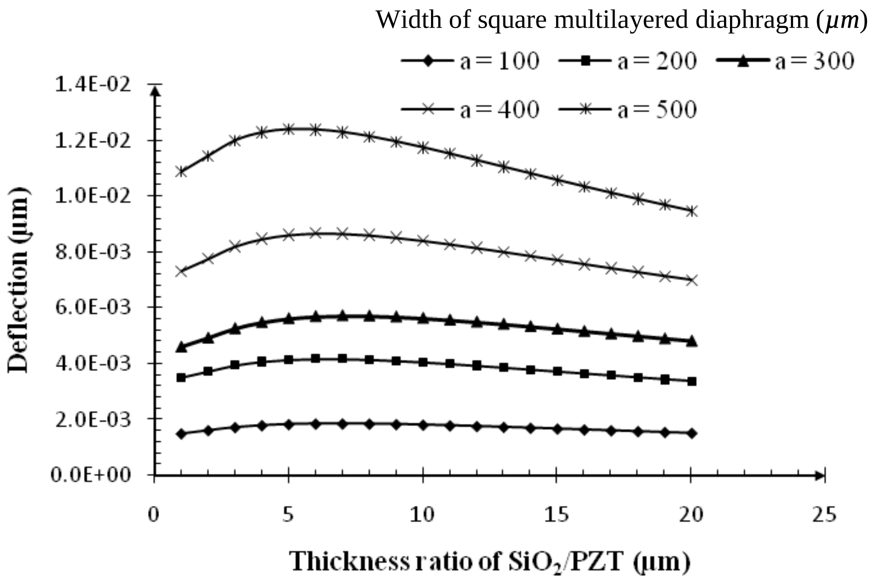

Fig.11. Dependence of the diaphragm deflection via the thickness ratio of SiO_2/PZT layers of the diaphragm

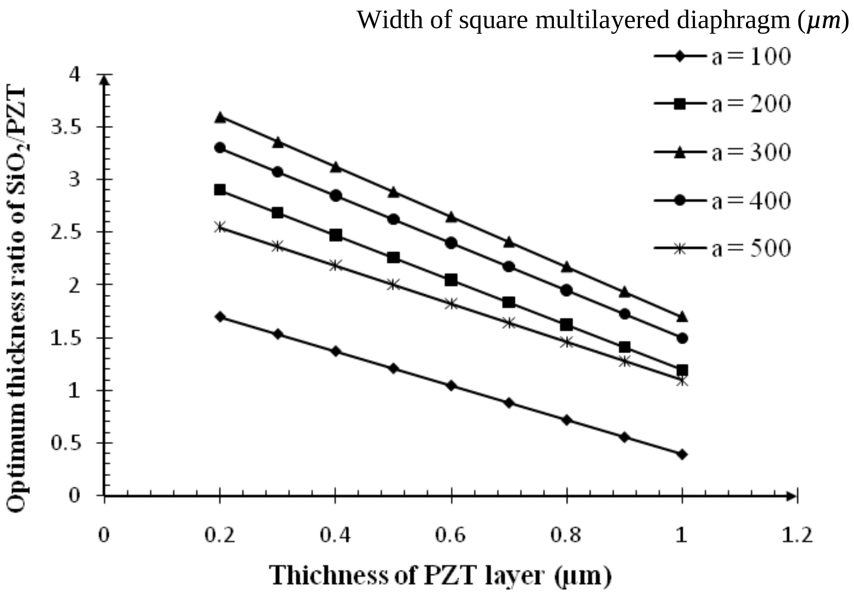

Fig.12. Change of optimum thickness ratio of SiO_2/PZT plate versus variation of PZT thickness and diaphragm width

4.4. Sensor response

Fig.13 shows the voltage versus pressure diagram for different diaphragm widths. In this diagrams the PZT layer thickness is constant and equal to 1 µm and the SiO_2 layer thickness is so selected to obtain the optimum value of R in that diaphragm width. These curves can be used to calibrate the sensor actuator response. There is a simple linear relation between voltage and pressure in each diaphragm width. This linear relation can be used to predict larger model behavior and calibrate them.

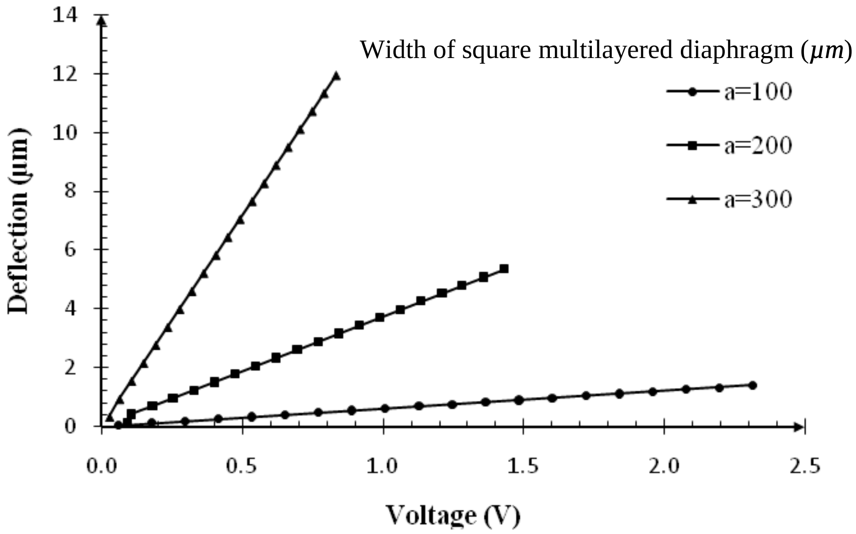

Fig.13. Diaphragm deflection versus voltage for different diaphragm widths

5. Conclusions

In present work, design, modeling and optimization of a pressure sensor is presented. The dynamics characteristics and structural behaviors of the multilayer PZT diaphragm were investigated to obtain an optimum design of the PZT thin film diaphragm for use in the sensors and actuators applications. A simplified model is introduced which can model the diaphragm with negligible error. Some linear relation were introduced which can be used in the larger model. Using these relations will lead to save huge amount of CPU time and required hardware in further studies. It was shown that there is a linear relation between the first natural frequency and PZT layer thickness, first natural frequency and reciprocal area of diaphragm, voltage and pressure curve. The deflection at center point of diaphragm as a function of the thickness ratio of PZT layer to SiO_2 layer, R, was presented. The optimum R value was obtained for different PZT layer thicknesses for the optimum design of actuator or sensors in MEMS applications.

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