The Sixth International Workshop on Micro and Nanotechnology for Power Generation and Energy Conversion Applications, Nov. 29 - Dec. 1, 2006, Berkeley, U.S.A.

A Comparison of piezoelectric materials for MEMS power generation

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Abstract

The performance of AlN, ZnO, PZT, and PMN-33%PT as active layers in a piezoelectric device for energy conversion is examined in the context of electromechanical coupling coefficient. A figure of merit based on materials properties is used to identify PZT and PMN-33%PT as the most promising candidates. A full finite element model is then implemented to compare the performance of the PZT and PMN-33%PT. The results show that for the configuration selected PZT delivers the highest energy conversion efficiency.

Keywords: PowerMEMS, Piezoelectric, Electromechanical coupling, Efficiency

1 - INTRODUCTION

Piezoelectric materials are increasingly proposed as a means to convert mechanical to electrical energy in small scale systems. Lead zirconate titanate, (PZT), is the active piezoelectric material in the majority of energy conversion devices reported in the literature [1-9]. There are however, several other candidate materials including single crystal PMNPT, PVDF, $LiNbO_3$, AlN, and ZnO. In this work the relative merits of alternative materials will be evaluated in the context of power generation.

In previous work we have shown that the efficiency of energy conversion of a piezoelectric device is strongly dependent upon the electromechanical coupling coefficient and that the coupling coefficient depends strongly on process and design parameters [8 -10]. Material properties such as $d_{31,}$ the stress based piezoelectric coefficient and $\varepsilon^{\tau}_{33,}$ the dielectric constant, have a direct effect on the electromechanical coupling coefficient. In addition to materials properties, for MEMS devices the characteristics of the composite structure such as residual stress, side length, aspect ratio, electrode coverage, layer thicknesses, and boundary conditions also have a substantial impact on electromechanical coupling [9-11].

The geometry studied in this work is that of a piezoelectric diaphragm that is used to convert mechanical to electrical energy in a micro heat engine [1]. In the past we have focused on the use of PZT as the active piezoelectric material. In this work we examine the merits of alternative active layers. In particular, a comparison of AlN, ZnO, PZT and PMNPT is made.

2 - CANDIDATE MATERIALS

The salient properties of the materials selected for comparison are shown in Table 1. As noted, PZT is a popular choice for energy conversion applications. The properties of the PZT listed are representative of thin film 52:48 PZT produced in-house [9,10]. ZnO is widely used as a transducer material in mechanical sensors [12]. Aluminum nitride is a well-established material for thin surface acoustic wave applications [13]. Single crystal PMNPT is an attractive candidate due to its very high d_{31} values. Both single-domain and multi-domain PMN-33%PT material properties are listed [14].

Table 1 – Candidate Material Properties

	d_{31} (-)10-12 C/m^2	ε^{τ}_{33} ε_o	s_{11}^E 10-12 m^2/N
AlN	1.5	10.5	2.9
ZnO	2.2	4.6	7.7
PZT	88	1000	12.1
PMN-33%PT (Multi)	1335	8200	70.5
PMN-33%PT (Single)	90	640	62.2

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In previous work a one-dimensional model of plate/membrane behavior was used to derive an expression for the electromechanical coupling coefficient for a simply supported diaphragm [9]. A simplified version of the expression is shown below.

$$k^2 = \approx \frac{1}{E_{sub}} \frac{\left(d_{31}/s_{11}^E\right)^2}{\varepsilon_{33}^T\left(1-\frac{d_{31}^2}{s_{11}^E\varepsilon_{33}^T}\right)}\{Geometry\} \qquad (1)$$

The electromechanical coupling coefficient depends on the materials properties d_{31}, ε^{τ}_{33}, and s_{11}^{E} (mechanical compliance). The stiffness of the substrate (E_{sub}) is also important. Important geometric parameters include layer thicknesses and the neutral axis position. The details may be found in [9].

Given that the geometry may be optimized for any given active layer on a common substrate such as silicon, the above expression may be used to provide an estimate of the relative performance of a candidate active material. The term in the bracket in the denominator is essentially unity and so one may compare materials on the basis of the ratio

$$(k^2)^* = \approx \frac{\left(d_{31}/s_{11}^E\right)^2}{\varepsilon_{33}^T} \qquad (2)$$

Examination of these properties in Table 1 reveals striking differences between the materials. For example the d_{31} value for the multi-domain PMN-33%PT is the highest of all the materials. However, this material also has the highest ε^{τ}_{33}, and s_{11}^{E}. The single domain PMN-33%PT is comparable to the PZT in terms of d_{31} and ε^{τ}_{33}; however, s_{11}^{E} of the single crystal material is substantially higher. Although the d_{31} of AlN is quite low the relatively low value of ε^{τ}_{33} has the potential to offset this deficit. The ratios $(k^2)^*$ for each of the material were calculated and compared to that of PZT as a standard of comparison. The results are shown in Table 2.

Based on this analysis one could conclude that PZT is the superior material. Certainly this seems reasonable for both ZnO, AlN, and the single-domain PMN-33%PT which produce coupling coefficients far below that attainable with PZT. However the expressions shown in eqns 1 and 2 are based on a 1D analysis of an element in pure bending. In reality the structures of interest are three dimensional and subjected to bending and stretching. For further evaluation we turn to the use of a FE model to compare the performance

Table 2 – Relative Electromechanical Coupling

PZT	AlN	ZnO	PMNPT (multi)	PMNPT (single)
1	0.47	0.34	0.85	0.6

of a diaphragm with PZT as the active material and PMN-33%PT as the active material.

3 - RESULTS

The commercial finite element package ABAQUS/Standard (2004) is used. The piezoelectric model has been implemented as a user element subroutine for a triangular membrane element. The non-piezoelectric layers are modeled as triangular general-purpose shell elements. Details of the code and its implementation may be found in [15].

Figure 1 shows a cross section of the geometry modeled. In the figure is shown the configuration for the PZT device,

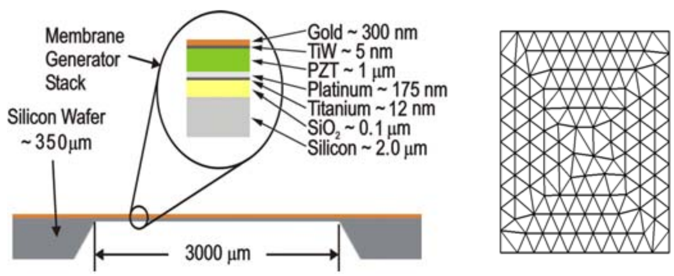

Fig. 1. Geometry of device and mesh.

which consists of a silicon membrane, a bottom platinum electrode, a thin-film of the piezoelectric ceramic PZT and a top gold electrode. Devices like this have been fabricated and tested extensively [10]. For comparison the same laminate geometry is used for the PMN-33%PT; that is, only the active layer properties are changed. The mesh is also shown in the figure. The mechanical properties and thicknesses of the layers are shown in Table 3.

The code has been validated with experimental data obtained on the PZT device. The modeled and experimental mechanical and electrical behaviors are shown in Fig 2. The midpoint deflection of the diaphragm is versus applied pressure showing the mechanical response.

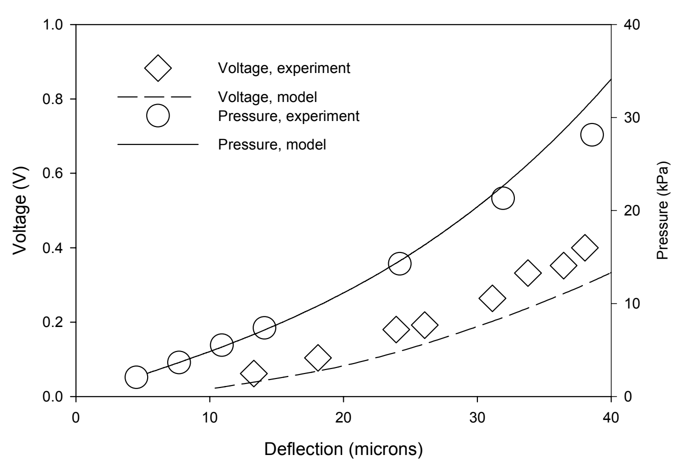

Fig. 2 Comparison of model and experiment.

Table 3. Properties of the layers of the laminate.

Material	Modulus, E, GPa	Poisson's ratio, ν	Density, ρ kg/m3	Thickness μm
Si	160.0	0.27	2330	2.00
SiO_2	72.1	0.17	2200	0.10
Ti	129.0	0.32	4510	0.0125
Pt	203.0	0.39	21100	0.175
PZT	74.7	0.25	7500	1.25
TiW	129.0	0.41	19000	0.005
Au	94.7	0.42	19400	0.30

The open circuit voltage is plotted versus the midpoint deflection of the diaphragm.

To assess device performance in a power generation application, the code is run in a closed circuit condition. The efficiency of power conversion is the ratio of the electrical power delivered to a load resistor and the total input mechanical power. The load resistor is varied to find the optimum load for power transfer (i.e. impedance matching). Modeled efficiency versus load resistance results are shown plotted in comparison to experimental data in Fig. 3. The code predicts the experimental results well.

To compare the performance of a thin film PZT diaphragm as a power generator to that of a PMN-33%PT diaphragm

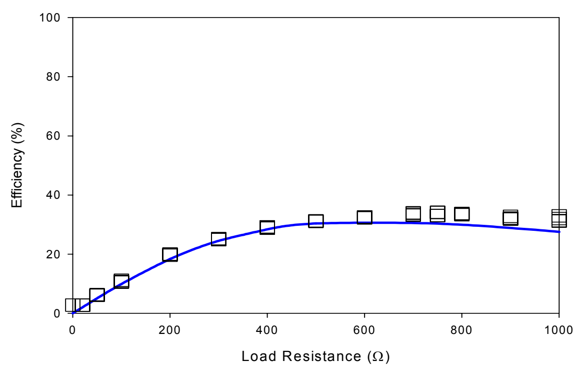

Fig. 3. Modeled efficiency compared to experimental efficiency.

laminates consisting of a 2 micron silicon substrate with 1.25 microns of active material were modeled. The electrode layers were of the same dimensions as shown on Fig. 1. The diaphragms were 3 microns on a side. The electrodes were centered on the diaphragm and covered 60% of the total area. The results are shown in Fig. 4. The results show that the PZT diaphragm is the most efficient followed closely by the multi-domain PMN-33%PT.

Thus the initial estimate of performance provided by equation 2 has held. However, the ratio between the active material thickness and the substrate material thickness is important for optimal electromechanical coupling [15]. In the simulation the thickness of the active material was held constant at 1.25 microns. A plot of electromechanical coupling versus the

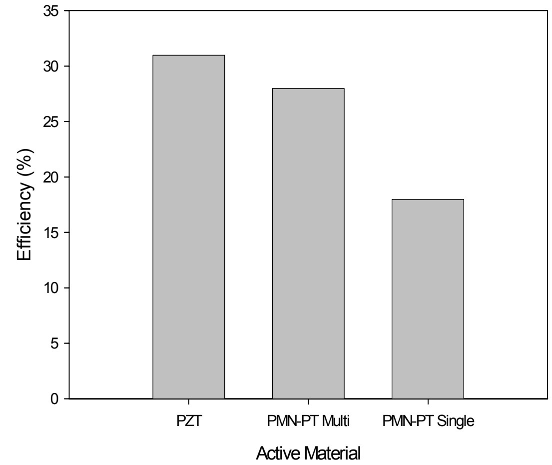

Fig. 4. Predicted efficiencies of PZT and PMNPT devices.

ratio of active layer thickness to substrate thickness is shown in Fig 5 for the PZT and PMN-33%PT. As shown in the figure the optimum thickness ratio for a PZT diaphragm is about 0.25 whereas for a PMN-33%PT diaphragm it is closer to 1. For a more equitable comparison optimal configurations for each of the materials should be devised. In the case of the PMN-33%PT a change of substrate material may be required to realize a practical device configuration. Referring back to equation 1 it can be seen that the substrate thickness has an effect on the electromechanical coupling coefficient. In general, a stiffer substrate will lead to higher coupling coefficient; if the thickness ratio is optimized. In future work we will develop a practical device configuration for comparison to the PZT device.

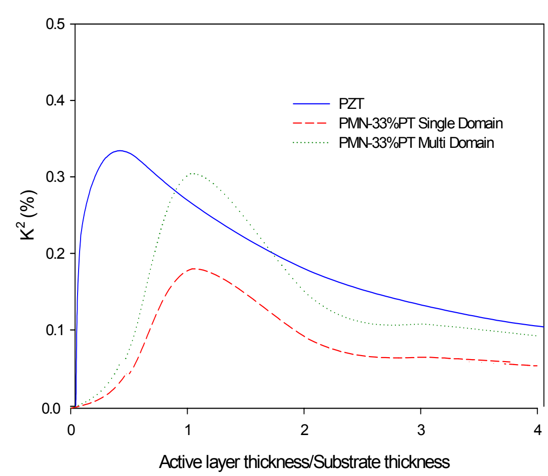

Fig. 5. Coupling coefficient as a function of active layer to substrate thickness.

4- SUMMARY

The materials AlN, ZnO, PZT, and PMN-33%PT were considered as potential candidates for the active layer in a device for the conversion of mechanical to electrical energy. A figure of merit based on materials properties was used to identify PZT and PMN-33%PT as the most promising candidates. A full finite element model was then implemented to compare the performance of the PZT and PMN-33%PT as active layers in a laminate structure. The results show that for the configuration selected PZT delivers the highest energy conversion efficiency. Future work will focus on identifying the optimal configuration of a device with each of the materials for further comparison.

ACKNOWLEDGMENTS

Financial support was provided by the US Army SMDC under contract #DASG60-02-C0001.

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