A STUDY ON EPITAXIAL PIEZOELECTRIC THIN FILMS GROWN ON SILICON FOR ENERGY SCAVENGING APPLICATIONS

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Abstract: This paper presents the design, analysis and fabrication of a MEMS energy scavenger based on an epitaxial $Pb(Zr_xTi_{1-x})O_3$ (PZT) thin film grown directly on a silicon substrate. A focus is dedicated to the characteristics of the epitaxial PZT film, composition and thickness, for an optimum power generation, and especially to the modeling, design and optimization of an epitaxial PZT cantilever beam with a proof mass. Different parameters including beam dimensions, proof mass and output power are optimized through computational simulation and theoretical analysis. The calculated output power generated by the epitaxial PZT cantilever with a Ni proof mass whose resonant frequency is around 70 Hz can reach to up to 1 μW at 33 kΩ of load resistor. Microfabrication processes with an associated process flow to fabricate the epitaxial piezoelectric cantilevers are also presented.

Key words: epitaxial films, piezoelectric MEMS, energy scavenger, PZT microcantilever

1. INTRODUCTION

MEMS based energy scavengers are attractive as an alternative power source for low-power electronic devices and sensors, with as one of their potential applications, their implementation in wireless sensor nodes. The development of scavengers to generate energy from vibrations has advanced rapidly during the past few years. Several transduction methods are under investigation including electromagnetic induction, electrostatic generation, and piezoelectric materials. Among these methods, piezoelectric materials have received the most attention due to a higher power density which shows higher energy conversion efficiency. Several bulk and thin-film piezoelectric energy scavengers have been reported so far, but there has been scarcely high quality thin-film piezoelectric energy scavenger in the scale of MEMS.

Epitaxial piezoelectric (epi-piezo) thin films are perfect candidates for vibrational energy scavenging applications as they exhibit an efficient high vibration-to-electricity conversion. Their properties, including the piezoelectric coefficients, polarizations, and dielectric constants can be superior to polycrystalline piezoelectric films [1]. We have demonstrated that epi-piezo thin films can be grown on silicon through oxide transition layers. These piezoelectric films are atomically smooth and exhibit microstructural homogeneities [2]. Moreover, the epitaxial growth of piezoelectric thin films on the oxide layers can reduce the fatigue effect and cyclic depolarization, which is necessary for a reliable use in future devices. The successful combination of epi-piezo thin films on silicon substrates with microfabrication techniques allows the realization of MEMS with enhanced actuation/detection properties [3]. In this paper, we report on the integration of the epi-piezo thin films on silicon for vibrational energy scavenging applications. Different aspects related to the requirement for effective vibrational energy scavenging by the epi-piezo thin films are addressed: materials selection, epi-piezo films growth on silicon, micro-patterning methods, and especially design and optimization of the epi-piezo energy scavengers.

2. EPI-PIEZO THIN FILMS ON SILICON

2.1 Epitaxial Thin Film Deposition

To grow epitaxial thin films with robust piezoelectric response on silicon, we use a $SrTiO_3$ (STO) buffer layer grown by molecular beam epitaxy directly on 2” (100) Si wafers in order to chemically engineer the interface between silicon and the oxide [4]. Then, we grow by off-axis magnetron sputtering a $SrRuO_3$ (SRO) film used as a bottom electrode [5]. We choose $Pb(Zr_xTi_{1-x})O_3$ piezoelectric film as an active layer in our energy scavenging systems due to its high electromechanical conversion behavior. PZT thin films are grown by off-axis magnetron sputtering. The typical final stack results as PZT (200 nm)/SRO (30 nm)/STO (10 nm)/Si as shown in Fig. 1(a). X-ray diffraction analysis confirms the epitaxial relationship between the oxide layers and the substrate. Theta-2theta diffraction spectra (Fig. 1(b)) display only (001) peaks, confirming the *c*-axis orientation of the oxide stack. Local piezoelectric hystereses performed with an atomic force microscope exhibit ferroelectric behavior: the piezoelectric coefficient d_{33} is of the order of 80 pm/V and the coercive field is 2 V.

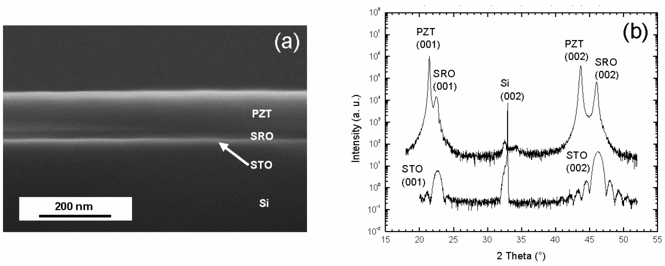

Fig. 1: (a) Cross-sectional SEM image of epitaxial PZT/SRO/STO thin films grown on a Si (100) substrate, (b) Theta-2theta diffraction scan.

2.2 Analysis of the Characteristics of the Epi-Piezo PZT films on Power Generation

To maximize the generated output power, a special attention needs to be given to the PZT composition and thickness.

The ratio of piezoelectric coefficient d_{31} over dielectric constant ε must be high to obtain high output power according to the analytical model reported in [6]

$$P = \frac{1}{2\omega^2}\frac{RC_b^2\left(\frac{1.5E_P d_{31} t_p\left(t_p + t_s\right)}{l_b^2 \varepsilon}\right)^2 A_{in}^2}{\left(4\zeta^2 + k_{31}^2\right)\left(RC_b\omega\right)^2 + 4\zeta k_{31}^2\left(RC_b\omega\right) + 4\zeta^2} \quad (1)$$

where R: resistive load, C_b: capacitance of the PZT film, E_p: Young's modulus of the PZT film, t_p: thickness of PZT, t_s: thickness of silicon, l_b: length of cantilever, A_{in}: acceleration of vibration source, ζ : mechanical damping ratio, k_{31}: coupling coefficient, and ω: the angular frequency of the vibration source which is equal to the resonant frequency of the cantilever.

Although, this equation was developed for a simple resistive load, it gives a reasonably decent estimation of the amount of power generated. The remanent polarization P_r, the dielectric constant ε and the piezoelectric coefficient d_{31} of the PZT films with different Zr/Ti ratios were studied in [7]. Based on these parameters, the normalized output power as the function of Zr content can be calculated from Eq. 1, and is illustrated in Fig. 2.

It shows a decrease in the output power with increasing Zr content of the PZT films. The Zr/Ti ratios play an important role in the power generation. Here, for the energy scavenging application, the $Pb(Zr_{0.2}Ti_{0.8})O_3$ piezoelectric film is our choice due to high ratio of piezoelectric coefficient d_{31} over dielectric constant ε, and also the good lattice match with STO and SRO [8].

Besides the PZT composition, the output power is also defined by the PZT thickness. The power generated, can be increased significantly by increasing the PZT thickness. However, presently the growth of our PZT thin films is limited to maximum thickness of 200 nm. An improved deposition method for thicker epitaxial PZT thin films is under investigation. An alternative that we are also considering is the use of PMN-PT, potential piezo characteristics and thickness.

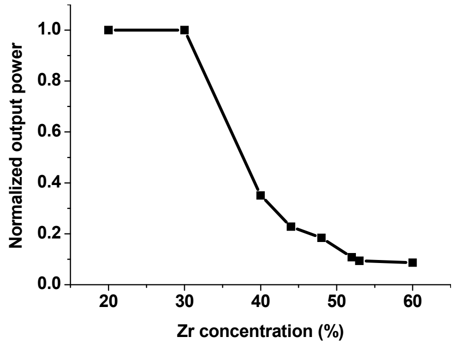

Fig. 2: Normalized output power as the function of Zr concentration based on parameters in [7].

3. MODELING AND ANALYSIS

The frequency range of the ambient vibrations of interest in our environment is in the order of 60-200 Hz [6]. The energy scavenging device needs to be designed to match such low frequency in order to achieve the maximum output power. A cantilever beam is the most compliant structure for a given input force. It can generate larger strain compared to bridge and diaphragm structures. The cantilever structure can be easily designed to have a low resonant frequency. Therefore, epitaxial PZT cantilever beam structures with an optional proof mass are investigated to scavenge the energy from the vibrations. The ultimate goal of epitaxial PZT cantilever design for energy scavenging applications is to have a low resonant frequency, high output power, and compactness in the scale of MEMS devices. Through computational simulation and theoretical analysis, we have investigated the design of the epi-PZT cantilevers, beam dimensions and proof mass, for an optimum power generation.

3.1 Resonant Frequency Analysis

The PZT cantilevers must exhibit a resonant frequency that matches the dominant frequency of a given ambient vibration in environment to maximize

Table 1: Materials' properties for FEM simulation.

SILICON	
Mass density (kg/m^3)	2330
Young's modulus (GPa)	120
Poisson's ratio	0.28
Thickness	1 to 50 um
PZT	
Mass density (kg/m^3)	7550
Relative permittivity matrix [ε_r]	$\begin{bmatrix} 638 & 0 & 0 \\ 0 & 638 & 0 \\ 0 & 0 & 583 \end{bmatrix}$
Stiffness matrix [c^E]$^{-1}$ (GPa)	$\begin{bmatrix} 119.0 & 57.9 & 56.0 & 0 & 0 & 0 \\ 0 & 119.0 & 56.0 & 0 & 0 & 0 \\ 0 & 0 & 110.0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 30.4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 30.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 30.5 \end{bmatrix}$
Piezoelectric matrix [e] (C/m^2)	$\begin{bmatrix} 0 & 0 & -2.67 \\ 0 & 0 & -2.67 \\ 0 & 0 & 11.31 \\ 0 & 0 & 0 \\ 0 & 7.65 & 0 \\ 7.65 & 0 & 0 \end{bmatrix}$

the power generation. The resonant frequency of PZT cantilevers with various dimensions was first simulated by finite element method (FEM) in ANSYS. The PZT cantilever consists of a PZT film stacked on a silicon beam. These two layers have the same geometry and dimensions but different thicknesses. The thickness of the PZT layer was fixed at 200 nm. The buffer and electrode layers were neglected for simplification. The material parameters used for the FEM simulation are listed in Table 1.

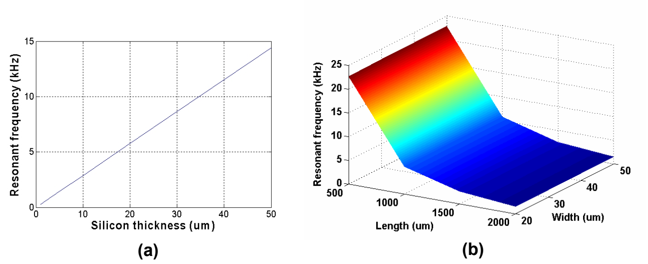

Fig. 3: Resonant frequency with respect to (a) the silicon thickness for a 50-µm wide and 2000-µm long cantilever, (b) the cantilever width and length for a fixed silicon layer of 5 µm.

Fig. 3(a) illustrates the first resonant frequency of the PZT cantilever as a function of thickness of silicon layer. It shows a decrease in the resonant frequency with decreasing the thickness. The resonant frequency as a function of thickness of its width and length, for a fixed silicon layer of 5 µm is also sketched in Fig. 3(b). It is obvious that longer and thinner PZT cantilevers must be designed to have a low resonant frequency which matches to the frequency of vibrations from the environment. Alternatively, we have evaluated the addition of a proof mass at the end of the cantilever that can reduce its resonant frequency while maintaining the compactness of the device.

3.2 Analysis of PZT Cantilever with a Proof Mass

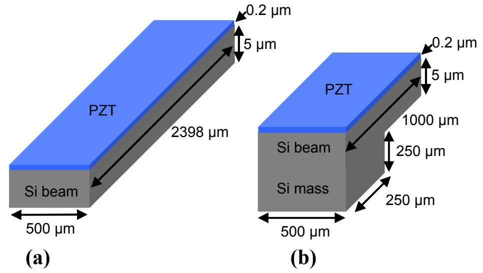

Fig. 4: Comparison of two PZT cantilevers (a) without a Si proof mass, (b) with a Si proof mass.

A comparison study of two PZT cantilevers without/with a Si proof mass has been carried out in ANSYS as modeled in Fig. 4. Both structures have the same resonant frequency around 1 kHz (modal analysis). Adding the Si proof mass results in a significant reduction of the cantilever length as expected. Harmonic analysis reveals that two PZT cantilevers have also the same maximum of deflection at the resonant frequency as shown in Fig. 5. If we apply the same deflection (13 µm) to both cantilevers, more induced voltage is generated in the cantilever with mass (33.727 mV) than in the one without mass (5.838 mV). These results imply that the PZT cantilever with a proof mass can generate higher induced voltage and hence output power than the one without a proof mass at the same resonant frequency due to heavier effective mass and stiffer beam.

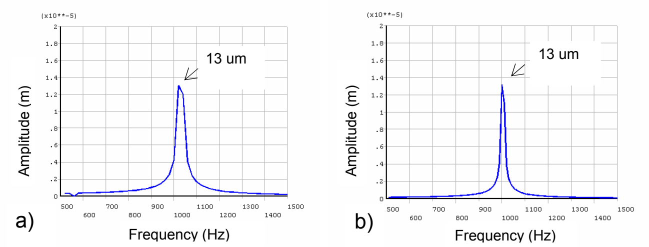

Fig. 5: Harmonic responses of PZT cantilevers (a) without a mass, (b) with a mass.

3.3 Output Power Analysis

The effective mass of the structure is a key parameter to design a compact MEMS energy scavenger as described in the previous subsection. To achieve a low resonant frequency and a high output power, a heavy proof mass is highly desirable. We have chosen nickel (Ni) as a material of proof mass due to higher mass density compared to silicon and SU8, for instance. The output power analysis of an epitaxial PZT cantilever with a Ni proof mass was performed based on Eq. 1. The physical parameters used for silicon and PZT are listed in Table 2. An acceleration A_{in} of 9.8 m/s^2 and a damping ratio ζ of 0.01 have been chosen as a baseline for comparison purpose.

Table 2: Parameters of Si and PZT for the analytical calculation of the output power.

	t (µm)	w (µm)	l (µm)	E (GPa)	d_{31} (pC/N)	k_{31}	ε_r
Si	5	1000	2000	120	-	-	-
PZT	0.5	1000	2000	80.65	70	0.23	585

The output power and the first resonant frequency of the PZT cantilevers as a function of weight of the Ni proof mass are illustrated in Fig. 6. It is clearly seen that adding a heavier proof mass does not only decrease the resonant frequency but also increases the power generation. The output power generated by the optimized epitaxial PZT cantilever with a 3.5 mg of Ni proof mass whose size is 1000 µm wide, 800 µm long and 500 µm thick can reach to up to 1 µW at 33 kΩ of load resistor. The resonant frequency is 70 Hz. Considering the total volume of the cantilever, the power density is around 2.5 mW/cm^3.

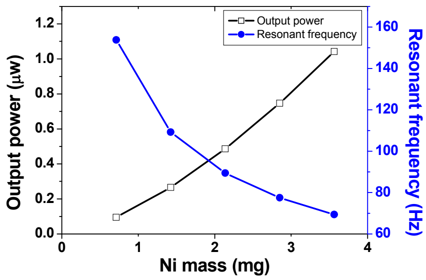

Fig. 6: Output power and resonant frequency as a function of Ni mass.

4. FABRICATION PROCESS

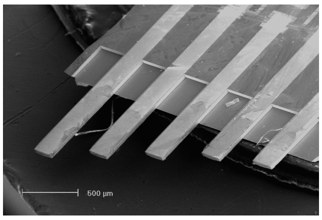

Fig. 7: SEM image of epitaxial PZT cantilever array.

In this section, we present the fabrication process of epitaxial PZT microcantilever arrays based on the developed micropatterning techniques presented in [3]. The fabrication sequence of the devices is described as follows. First, the STO buffer layer, the SRO bottom electrode and the PZT thin film are deposited on a 2" silicon substrate. Contact pads are opened through the epitaxial PZT films by a HF/HCl solution. The shape of the microcantilevers is then patterned through the PZT/SRO/STO stack by ion milling. The backside of the silicon wafer is etched by deep reactive ion etching (DRIE) to define the thickness of the structures. The Au/Cr is metallized for the top electrodes and electrical contacts for the bottom electrodes. We deposited and patterned the electrode at the end of the fabrication process to avoid the loss of ferroelectricity during the process. Finally, the structural release process is performed by DRIE from the top side of the wafer. The fabricated epitaxial PZT cantilever array as a first prototype is shown in Fig. 7. The beams are 50 µm thick, 200 µm wide and 200-1000 µm long at the moment. Testing of these epitaxial PZT cantilevers is underway to characterize their electrical and mechanical behaviors to validate the modeling performed.

5. CONCLUSION

We have reported on the design, analysis and fabrication of the epitaxial PZT microcantilever for energy scavenging applications. The PZT thin film has been grown epitaxially on silicon through the oxide layers, which shows good ferroelectric properties. The composition of the epitaxial PZT thin films and the geometry of cantilever beam with a proof mass were analyzed and optimized to achieve maximum power generation. The $Pb(Zr_{0.2}Ti_{0.8})O_3$ piezoelectric film was selected due to highest ratio of piezoelectric coefficient d_{31} over dielectric constant ε. The optimized epitaxial PZT cantilever can generate approximately 1 µW (2.5 mW/cm^3) at 70 Hz of resonant frequency. The rule of thumb for their design is to increase the effective mass of the structure by adding a heavy proof mass which can provide low resonant frequency, high output power and compactness, simultaneously. Finally, arrays of epitaxial PZT cantilevers were fabricated successfully and the characterization of their performances remains to be done, with and without proof mass. MEMS energy scavengers based on epitaxial PZT thin films are promising and could bring benefits such as superior performances and stability.

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