Modeling and Simulation of PVDF-TrFE Based MEMS Scale Cantilever Type Energy Harvesters

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ABSTRACT

In this paper, we present the FEM modeling and simulation of a cantilever type piezoelectric energy harvester (PEH) constructed using PVDF-TrFE. Frequency domain analyses are performed under a 10 µN tip force on the 2D model of a 600 µm-long cantilever, which consists of a 7.25 µm PVDF-TrFE layer on top of a 2 µm SiO_2 film. The same analyses are repeated using ZnO, AlN, and PZT-5A for comparison. Simulated maximum output powers and corresponding voltages are 60.3 nW at 0.73 V for PVDF-TrFE, 62.0 nW at 0.32 V for ZnO, 12.4 nW at 0.13 V for AlN, and 301.9 nW at 0.07 V for PZT-5A. The effects of a multi-layer approach on the device outputs are also simulated for PVDF-TrFE, which shows that the maximum output power is not affected by the number of layers. Our study demonstrates that PVDF-TrFE, a biocompatible piezoelectric polymer, can be easily used in a single or multi-layer architecture with no significant loss of power; making it an attractive material for energy harvesting.

Keywords: energy harvesting, PVDF-TrFE, piezoelectric

1 INTRODUCTION

Energy harvesting has become a widely studied research topic in the last decade. Probably the most important impetus for this interest is their potential to enable self-sustained electronic systems by eliminating the need for an external energy supply. Self-sustaining ability becomes more important for the applications where the access to the electronic system is limited or infeasible, such as wireless sensor networks (WSNs) or implantable medical devices (IMDs). The most convenient method to integrate a small-sized, lightweight, and efficient energy harvester to such electronic devices is to fabricate them monolithically on the same substrate using CMOS compatible MEMS techniques.

The most commonly used architecture for piezoelectric energy harvesting is the cantilever beam, which is used to harvest energy from ambient vibrations [1]. The essential components of a cantilever type piezoelectric energy harvester (PEH) are a structural layer, a piezoelectric layer, and metal electrodes. In addition, a proof mass is usually placed at the tip of the cantilever to reduce the resonance frequency and increase the stored mechanical energy.

PZT is probably the most widely preferred piezoelectric material in MEMS scale due to its high electromechanical coupling [2]. Although there are different PZT thin film deposition techniques such as epitaxial deposition or aerosol deposition, sol-gel is the most commonly used method. However, PZT films deposited using these techniques require a high temperature annealing step for crystallization; and therefore, they are not CMOS compatible. Another problem of PZT is its lead content, which makes it unsuitable for IMD applications. ZnO and AlN are two other piezoelectric materials used in MEMS scale piezoelectric devices. The most prominent advantage of these materials is that they can be deposited at low temperatures using sputtering, which makes them CMOS compatible. Furthermore, there are studies suggesting that both ZnO [3, 4] and AlN [5] are biocompatible. However, all these materials are brittle and have relatively high stiffness constants. High stiffness increases the resonance frequency of the structure, which is usually already high for MEMS scale devices, and brittle layers are more susceptible to failure during operation.

A possible alternative to these commonly used materials is piezoelectric polymers. PVDF-TrFE is a piezoelectric copolymer with a moderate electromechanical coupling coefficient. It can be deposited easily using spin coating up to several micrometers, and its crystallization temperature, which depends on the molar composition, is below 180 °C [6]. Low crystallization temperature and simple deposition process makes it a CMOS compatible material [7]. PVDF-TrFE is soft and flexible as most polymers; consequently, it is possible to utilize thicker piezoelectric layers in PVDF-TrFE based PEHs. Its biocompatibility has also been studied and verified previously [8], which makes this material especially attractive for IMDs. Another advantage of its simple deposition process is that it allows fabricating multiple electrode/piezoelectric layers, which can be utilized to adjust the device capacitance for a given total thickness. The fabrication and energy harvesting capability of a multi-layer PVDF-TrFE based flexible cantilever type device has recently been demonstrated [9].

In this study, we present the 2D FEM analyses of PVDF-TrFE based, MEMS scale, cantilever type PEHs operating in d_{31} mode. The next section presents the modeling and simulation of a PVDF-TrFE based, single piezoelectric layer PEH. Same analyses are also performed using ZnO, AlN, and PZT-5A for comparison. Section 3 presents the FEM simulation results of a multi-layer PEH approach using PVDF-TrFE, and Section 4 presents the conclusions.

2 SINGLE PIEZOELECTRIC LAYER

Figure 1 shows the constructed 2D model of the cantilever type PEH. Suspended part consists of a 600 µm-long cantilever with a 2 µm-thick SiO_2 structural layer, a 7.25 µm-thick PVDF-TrFE layer, and a 40 µm-thick Si proof mass. The anchor point is modeled with a 50 µm-thick Si block, and the device is surrounded with air in order to improve the accuracy of the electric field calculations. The third dimension of the model, depth, is set as 500 µm. To keep the complexity of the model at a low level, electrode layers are not modeled explicitly. Instead, they are modeled as two electrical terminals, one at the top and the other at the bottom surface of the piezoelectric layer. Typical electrode thicknesses for MEMS devices are usually on the order of 0.1 µm, which is much smaller compared to the thicknesses of the other layers. Therefore, exclusion of electrode layers is not expected to have a significant effect on the results. Electrode length is selected as 400 µm as illustrated in Figure 1, since 2/3 of the cantilever length is shown to be the optimal electrode coverage [10]. Defined electrical terminals are connected to a resistive load via the electrical circuit module of COMSOL in order to evaluate the performance of the simulated device.

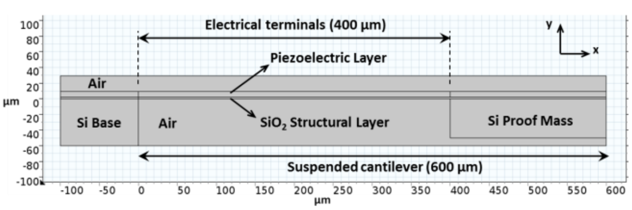

Figure 1: Constructed 2D model of the cantilever type PEH.

Performance of the PEH is investigated using frequency domain simulations. For this purpose, a 10 µN force is applied at the tip of the cantilever, and resistive load value is swept to reach the maximum output power. Excitation frequency is chosen such that the tip displacement is approximately 17 µm, which is a small enough value to allow using linear approximations. Figure 2 shows the simulated voltage distribution on the cantilever when it is excited with a 10 µN force at 3200 Hz, which results in a 17 µm tip displacement, and loaded with a 15 MΩ resistor.

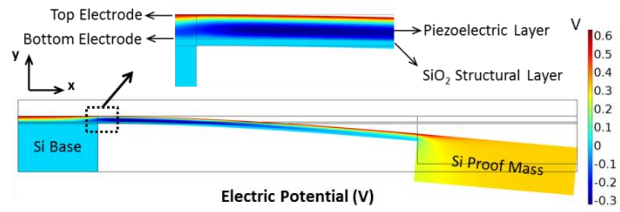

Figure 2: Simulated voltage distribution on the cantilever with a 10 µN tip force applied at 3200 Hz. A 15 MΩ load resistor is connected to the electrical terminals.

Performance of PVDF-TrFE as a piezoelectric energy harvesting material is compared with commonly used materials in piezoelectric MEMS, such as ZnO, AlN, and PZT-5A, using a similar set of simulations. In these simulations, all structural parameters except the piezoelectric layer thickness are kept constant. Piezoelectric layer thickness is adjusted for each material such that the neutral axis of the cantilever stays at the same position. Neutral axis is defined as the plane with zero stress in a bent cantilever; stress is compressive on one side of the neutral axis and tensile on the other side. Cantilever type PEHs are designed to keep the neutral axis outside the piezoelectric layer as illustrated in Figure 3, in order to prevent charge cancellation because of the sign change in the stress. Therefore, the neutral axis position is chosen as 1.8 µm from the bottom surface of the 2 µm-thick SiO_2 layer throughout this study.

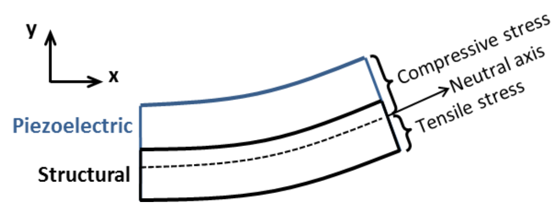

Figure 3: Illustration of neutral axis position in a cantilever type PEH.

The excitation frequency is also adjusted for each material while maintaining the 10 µN tip force such that the tip displacement is 17 µm. Finally, load resistance values are swept in different ranges for each material to find the optimum value, which results in maximum output power. In these simplified simulations, optimum load resistance is determined by the capacitance of the device and the operating frequency. For a constant operating frequency, optimum load resistance should decrease as the device capacitance increases. Table 1 lists the thickness, excitation frequency, and load resistance ranges used in simulations for different piezoelectric materials. As seen in the table, thickness values for other materials are much smaller in comparison to PVDF-TrFE. This is an expected result since the neutral axis tends to shift towards the stiffer material in a bilayer structure. Optimum load resistance values are also significantly different. On one end, the capacitance of PVDF-TrFE device is much smaller due to increased electrode distance, and this leads to higher optimum load resistance values. On the other end, optimum load resistance range is three orders of magnitude lower for the PZT-5A device compared to PVDF-TrFE device. This is because of the reduced electrode distance and high permittivity of PZT.

Material	Thickness	Freq.	Resistive Load
PVDF-TrFE	7.25 µm	3200 Hz	(12.0 - 23.5) MΩ
ZnO	1.00 µm	1748 Hz	(2.6 - 4.2) MΩ
AlN	0.60 µm	1605 Hz	(1.9 - 3.7) MΩ
PZT-5A	1.48 µm	1870 Hz	(30 - 38) kΩ

Table 1: Thickness, excitation frequency, and load resistance ranges used in simulations for different piezoelectric materials.

Figure 4 shows the simulated output powers and voltages for PVDF-TrFE, ZnO, and AlN. Peak output powers and corresponding voltages are 60.3 nW at 0.73 V, 62.0 nW at 0.32 V, and 12.4 nW at 0.13 V. These results show that piezoelectric energy harvesting performance of PVDF-TrFE is comparable to that of ZnO, and it is significantly higher than AlN. In comparison, PZT-5A gives 301.9 nW at 0.07 V under the same conditions. Although this power level is much higher than the other piezoelectric materials, it should be noted that the model parameters of PZT-5A are valid for bulk PZT, which has a much higher electromechanical coupling compared to thin film PZT. Therefore, a thin film PZT layer would result in a lower power output.

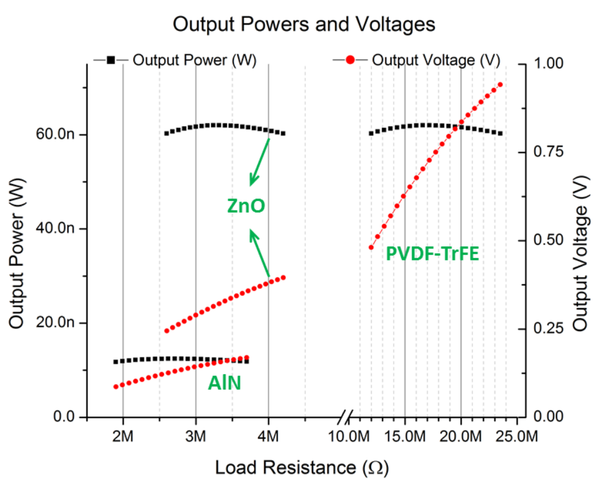

Figure 4: Simulated output powers and voltages for PVDF-TrFE, ZnO, and AlN.

3 MULTIPLE PIEZOELECTRIC LAYERS

FEM simulations presented in the previous section shows that the low elastic constant of PVDF-TrFE allows utilization of thicker piezoelectric films. Its deposition process is also fairly simple; PVDF-TrFE layers up to several µm thicknesses can be deposited in a single spin coating. However, increased piezoelectric layer thickness leads to high optimum load resistance values. A possible method to overcome this problem is using multiple piezoelectric/electrode layers. This method allows utilizing a thick piezoelectric layer while keeping a relatively high device capacitance, which reduces the optimum load resistance. Fabrication of such multi-layer PVDF-TrFE devices has recently been demonstrated [9].

In the second part of the study, the performance of multi-layer approach on a PVDF-TrFE based PEH is investigated. For this purpose, piezoelectric layer is divided into 2, 3, and 4 layers while keeping the total thickness constant at 7.25 µm. Electrodes are again modeled only in the electrical domain. Figure 5 illustrates the electrode arrangements and poling directions used for multi-layer PVDF-TrFE approach. The alternating poling and electrode arrangement adds up the effects of each piezoelectric layer and creates parallel capacitors. Since the capacitance of each layer is also increased due to decreased electrode spacing, overall device capacitance is proportional to the square of the number of layers. Therefore, the capacitance of the 4-layer arrangement is 16 times the capacitance of the single layer arrangement.

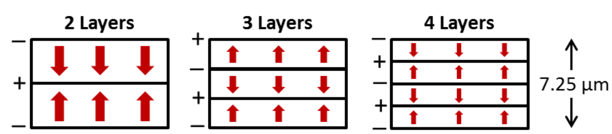

Figure 5: Illustration of the electrode arrangement and poling directions used for multi-layer PVDF-TrFE architecture.

Multi-layer approach does not significantly change the resonance frequency of the device since the total piezoelectric layer thickness is kept constant and electrode layers are not modeled in the mechanical domain. Therefore, simulations are run at the same frequency, which gives the same 17 µm tip displacement for each architecture. Figure 6 shows the simulated output powers and voltages for different number of PVDF-TrFE layers. The results show that the output voltage decreases with increasing number of layers while the total power stays constant at 60.3 nW. The voltage between two electrodes is equal to

$$V = \int \vec{E} \cdot \vec{dl} \quad (1)$$

where E is the electric field and dl is the infinitesimal length element. Therefore, reduced electrode distance decreases the output voltage. On the other hand, the capacitance increases with decreasing electrode distance, and this trade-off provides a constant output power. Since the simulations are run at a constant frequency, optimum load resistance is inversely proportional to the capacitance.

Consequently, multiple layers can be utilized to adjust the optimum load resistance without reducing the obtained power.

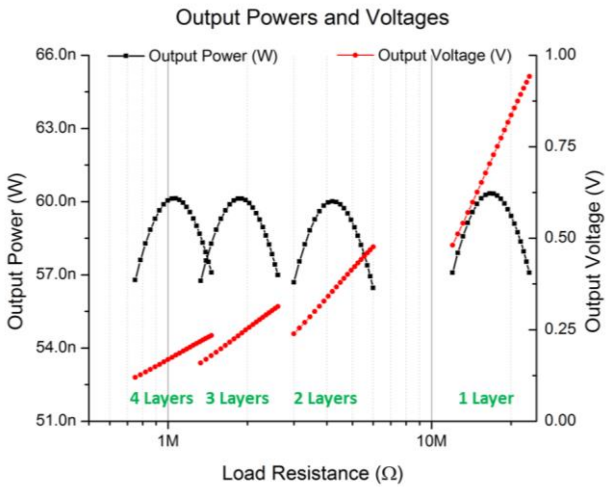

Figure 6: Simulated output powers and voltages for different number of PVDF-TrFE layers.

4 CONCLUSION

In this study, the performance of PVDF-TrFE for piezoelectric energy harvesting is investigated. PVDF-TrFE is a biocompatible, flexible, piezoelectric polymer that can be deposited on Si substrates using spin coating. Furthermore, its low crystallization temperature and simple fabrication process makes it a CMOS compatible material. FEM simulation results show that the energy harvesting performance of PVDF-TrFE on a cantilever type PEH is comparable to ZnO and higher than AlN. The performance of multi-layer PVDF-TrFE based cantilever type PEHs is also studied. Simulation results show that the output power is not significantly affected by a multi-layer approach as long as the total piezoelectric layer thickness is kept constant. On the other hand, it is possible to use the multi-layer architecture to adjust the output voltage levels, capacitance, and optimum load resistance of the device. With all these advantages, our study demonstrates that PVDF-TrFE is a promising material especially for flexible and MEMS scale PEHs.

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