Design considerations to enhance the performances of thin circular piezoelectric energy harvester diaphragms in harsh liquid environments

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Abstract. Thin circular piezoelectric energy harvester diaphragms undergoing large deflection in a harsh liquid environment are investigated in this paper. A material set combining AlN as transducer, SiC as electronics, Mo as wiring and Si as holder is considered. A highly accurate analytical model, which presents less than 5% error compared to FEM simulations in COMSOL, is first developed to study thoroughly flat diaphragms. Consequently, etching the wafer and adding a corrugation are proposed to reduce both the stress concentration at the edge and the influence of residual stress on the device behavior, respectively. Both ideas are predicted to increase the power density compared to the standard flat case by at least a factor of 5 to 10.

1. Introduction
Several monitoring applications necessitating MEMS technologies are operating under hostile conditions; specifications which make it impossible to consider deploying wired and battery-powered silicon devices or accessing them once disposed. These characteristics are typically encountered in geothermal wells, in oil/gas exploration, in gas turbines or in automotive/jet engines where temperature of 600 °C, pressures of 300 atm, shocks of 50’000 G and pH between 1 and 10 are common. Hence, solutions incorporating high robustness to a wide range of operating conditions and presenting almost an infinite lifetime are required; one of the reason for energy harvesters coupled with wireless sensor networks using wide bandgap semiconductors to become recently a topic debated in the field of microsystems [1, 2]. Therefore, intensive research is conducted in Pisano’s lab to create a micro-scale autonomous telemetry platform using aluminum nitride (AlN) as transducers and silicon carbide (SiC) as electronics. Inertial, pressure or temperature sensors [3, 4, 5], radio-frequency components [6], electronic circuits [7] and energy harvesters [8] based on this material set have been successfully fabricated.

In this work, a novel approach to design the most efficient thin circular piezoelectric energy harvester diaphragm vibrating in a liquid environment is proposed by combining theoretical modeling and FEM simulations in COMSOL. First, given a set of initial specifications, the dimensions of the standard flat structure are optimized thanks to an accurate analytical model. Then, two novel concepts to improve the global performances of the system are confronted: etching the wafer to reduce the stress concentration at the edge and adding a corrugation to modify the stress repartition within the diaphragm.
2. Theoretical modeling

Thin and flat circular piezoelectric energy harvester diaphragms driven by low frequency liquid pressure pulsations are studied. The design, illustrated in Figure 1, is divided into two models: a mechanical and an electrical one (both being related together thanks to the piezoelectric constitutive laws [9]). The mechanical analysis considers a bi-layer structure with an internal stress $T_0$, a radius $a$ and an overall thickness $h$ supported by uniformly distributed springs ($k_r$, $k_\theta$, $k_z$) at the edge and driven by an harmonic pressure load of amplitude $p_0$ and frequency $f_e$. The fluid-structure interaction is represented by a thin massive layer $m_f$ added on the surface. The equivalent electrical circuit is composed by four nodes ($i = 1, 2, 3, 4$) connected to the ground (GND) through pure capacitors $C_i$ emulating the piezoelectric material and pure resistive loads $R_i$ transforming the generated current $I_i$ into a voltage $V_i$.

2.1. Design methodology

The design methodology, reported in Figure 2, is built on several existing theories including notably large deflections of circular diaphragms [10, 11], piezoelectric energy harvesters [12, 13] and fluid-structure interactions [14]. Firstly, given the characteristics of the studied device and the environmental conditions, the tension parameter $K$ and the boundary conditions are set [10]. Secondly, the nondimensional spatial functions $W(\xi)$ and $S_r(\xi)$ are calculated [10, 11]. Thirdly, the nondimensional added virtual mass incremental (NAVMI) factor $\Gamma$ and the corresponding added mass $m_f$ are found [14]. Fourthly, the temporal function $\Phi(t)$ is obtained [12]. The three first steps are iterated a second time by substituting the tension parameter $K$ by the equivalent tension parameter $K_E$ accounting for the midplane tension to calculate the deflection $w$, the radial force $N_r$ and the radial displacement $u_r$ [10, 12]. Fifthly, the amount of stress-charges $Q_i$ generated on each electrode is derived [12]. Sixthly, the optimal load $R_{opt,i}$ and the open-circuit voltage $V_{oc,i}$ are found [12]. Finally, the total power recovered $P_{tot}$ is obtained by summing the maximal power $P_{opt,i}$ recovered by each electrode [13].
2.2. Model validation
In order to estimate the accuracy of the analytical model, FEM simulations have been implemented in COMSOL. An energy harvester with an overall thickness $h$ of 5 $\mu$m, a radius $a$ of 500 $\mu$m, a residual stress $T_0$ of 100 MPa and an excitation frequency $f_e$ of 60 Hz is reported as an example. The percentage of error between the theoretical model and COMSOL is illustrated in Figure 3. Errors of less than 5% were obtained over a broad range of pressures $p_0$ going from 0.1 atm to 10 atm, demonstrating the interest for implementing twice the mechanical model to account simultaneously for bending and stretching within the diaphragm. Additional iterations are useless, since they demand more computations without lowering significantly the error.

3. Further proposed improvements
Using our theoretical model, it was observed that the best piezoelectric energy harvester is a hinged symmetrical bimorph structure having the least amount of residual stress and two optimal electrodes patterned on either side. In order to emulate this design and thereby improve the global performances of the system, two concepts showing significant improvements compared to the standard flat diaphragm are proposed: etching the wafer and adding a corrugation. These advanced structures are illustrated in Figure 4 and were modeled using COMSOL.

3.1. Wafer etching
The goal of etching the wafer is to lower the high stress concentration at the edge by rendering it more flexible, while enhancing the output power and allowing rotation alike in a pinned edge situation. In fact, reducing the stress at the outer radius authorizes to fabricate wider diaphragms for a given maximal stress $T_{\text{max}}$ (usually the tensile strength of the material). This approach differs from the conventional ones, since, instead of modifying the design of the active device, the shape of the holder is engineered. In order to compare several manufacturing processes, two parameters have been defined: $\alpha$ which is the ratio between the initial radius of the reference device and the corresponding one of the novel energy harvester (remember both are presenting the same maximal stress $T_{\text{max}}$ at the anchor) and $\beta$ which is the ratio between the lateral etching rate and the vertical one.
For the studied case, an enhancement factor $G$ of almost 7 in terms of power density is expected at a pressure of 1 atm by using a simple wet isotropic etching step ($\beta = 1$). Better performances can be obtained by using highly anisotropic etching processes ($\beta > 1$), but they require a more complex fabrication. These observations are reported in Figure 5.

3.2. Corrugation

The behavior of thin and flat diaphragm are highly sensitive to environmental fluctuations. By adding a single corrugation of depth $d$ at the outer edge, the stress repartition within the structure is modified [15], resulting in performances stable over a wider range of temperatures and pressures. Actually, the presence of a corrugation generates a non-uniform stress [15] which allows lateral displacement, stretches the midplane and thereby creates additional charges. Meaning that under small deflections where bending is dominating (i.e. low pressure or high tensile stress), the performances are enhanced and that under large deflections where stretching is dominating (i.e. high pressure or low tensile stress), they are slightly reduced. Hence, more power can be recovered by a structure operating at low pressure in its tensile mode; a configuration commonly encountered.

For the studied case, with a residual stress $T_0$ of 100 MPa, a pressure load $p_0$ of 1 atm and a deep corrugation ($d/h > 5$), an enhancement factor $G$ of almost 6 in terms of power density is obtained. These results are given in Figure 6 in which several values of pressure and residual
stress are implemented. Each curve compares the performances of the corrugated diaphragm with respect to the flat one.

![Figure 6](image.png)

Figure 6: Improvements obtained by adding a corrugation. (a) Influence of the corrugation depth and the pressure load on the performances at a residual stress $T_0$ of 100 MPa. (b) Influence of the corrugation depth and the residual stress on the performances at a pressure load $p_0$ of 1 atm. Both red continuous lines are representing the same case.

4. Conclusion

A novel theoretical model to design thin circular diaphragm piezoelectric energy harvester has been reported and compared to FEM simulations in COMSOL for validation. Consequently, two concepts have been proposed to improve the global performances of the system. By judiciously choosing between isotropically etching the wafer or adding a corrugation, an enhancement by a factor 5 to 10 in terms of power density is obtained.

In the future, the new proposed ideas should be considered for the next generations of energy harvesters and several devices should be fabricated to properly validate the design methodology. The wet isotropic etching is thought to be the most powerful solution for the short term, whereas the corrugations will probably gain importance in the future; once their fabrication will be better controlled and more reliable.

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