Design, modelling and simulation of a PZN-PT actuated micropump

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ABSTRACT

We present an optimization methodology for the design of a self-priming piezoelectrically actuated pump made of a Pyrex wafer bonded to silicon. This methodology maximizes volumetric displacement of the actuating membrane and consequently the maximum flow rate performance.

It is shown that maximum membrane deflection does not necessarily equal maximum volumetric displacement, thus a pump can be better optimized for maximum flow rate by maximizing the stroke volume rather than the maximum membrane deflection.

The use of a novel piezoelectric material, a PZN-PT crystal, is proposed for the actuation of the pump membrane instead of the more commonly used PZT-5H.

The importance of the geometry and relative size of the elements in the membrane/actuator system is investigated by means of finite elements analysis, demonstrating that a square membrane with circular actuator at a radius ratio of 0.9 emerges as the optimal design.

Keywords: micropump, piezoelectric, diffuser, PZN, FEM

1 INTRODUCTION

Microfluidic devices are making their way into more and more areas of science and engineering. Especially for analytical chemistry and biomedical assays there is an interest in small, portable equipment that can be used in the field. As a crucial element of any such system, a means for liquid propulsion has to be provided. This problem is being addressed by the development of micropumps.

A number of different pumping principles has been studied over the last two decades and recently been reviewed in [3]. One of the most popular types of pump exerts pressure on the liquid through a reciprocating membrane which is actuated by a piezoelectric driver. To achieve pumping with such a system, valves are needed at the inlet and outlet to make the flow directional. Valves which are shaped like diffusers have first been used by Stemme and Stemme [7] by exploiting their direction-dependent flow resistance. Such valves have no moving parts and are therefore interesting for handling suspensions of particles or cells. While a number of researchers have etched the diffusers in the plane of a silicon wafer [1], the work by Gerlach et al. [2] used anisotropic etching to make diffuser-shaped holes through a wafer.

In the modelling of such micropumps, the literature has mainly taken note of the central deflection of the membrane as if it was bent by a uniform pressure load. However, the dependence of the volume displaced by each pump stroke on the membrane geometry and deflection profile has not been studied before.

2 PUMP DESIGN

We describe the design and optimization of a circular, reciprocating membrane micropump with piezoelectric actuation and nozzle-diffuser valves.

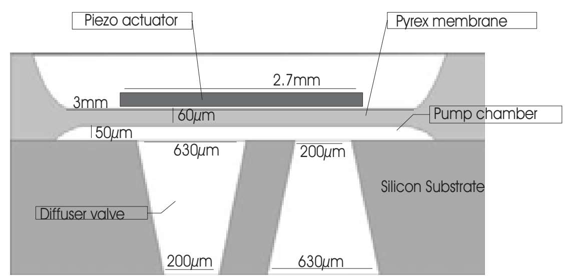

Figure 1 Diagram representation of the micropump, not to scale

2.1 The actuating membrane

The relationship relating a plate thickness to its diameter allows for optimization of maximum deflection. According to the measurement reported by Li in [6], the maximum achievable passive plate deflection reaches a peak when the passive plate thickness/diameter ratio is around 0.01–0.02; that is when the membrane is 50-100 times as large as its thickness.

A radius of 3mm and a membrane thickness of 60 µm were chosen for this design. Because of its excellent chemical and mechanical properties, Pyrex was chosen as the membrane material. Its coefficient of thermal expansion is close to that of silicon, and this allows for unproblematic anodic bonding of silicon-Pyrex structures.

Pyrex has a very high chemical resistance against water, acids, salt solutions, halogens and organic solvents. It has a Young's modulus of 67 GPa; this translates to a much larger deflection than that of silicon for a given actuation voltage for the piezo-electric element.

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2.2 The pump chamber

The pump chamber shape is dictated by the membrane shape and by the etching method. With a circular membrane, the pump chamber can be modelled - to a first order approximation - as an extruded circle, i.e. a cylinder. In reality, the isotropic etching of the Pyrex makes the pump chamber more like the frustum of a cone; however approximating its shape to a cylinder results in a quite acceptable 2% error (underestimation of volume).

The maximization of the *compression ratio*, dictates that the chamber volume to be minimized; hence, since the radius is a fixed parameter, the chamber height should apparently be reduced as much as possible. However Gerlach et al. in [2] suggests that a too shallow pump chamber negatively affects the flow through the diffusers. In the same paper it is established that the critical chamber height is a quarter of the smallest valve opening.

Since in this pump the nozzle and diffuser valve openings are 200 and 630 μm respectively, the critical chamber height results in 200/4=50μm.

2.3 The valves

While the shape of the valves is fixed by the KOH etching process of silicon which results in a truncated four-wall pyramid, their size, their number, and their arrangement within the pump chamber can be object of study and optimization.

KOH etching always attacks the silicon <100> plane creating an opening angle of 54.74 degrees. Given a set angle "of attack" and a set thickness of the wafer, the size of an opening on one side will result in a univocally smaller opening on the other side of the wafer.

It has been shown in [7] and [6] that the flow through the dynamic valves is not affected by the duct length or its larger opening as much as it is by its smaller opening.

From the experiments reported in [7] it appears that the optimum neck opening is 200 μm. A smaller value would increase the back pressure and negatively affect the maximum flow rate of the pump. At a larger value, the backpressure and flow rate dependence cease to be significant; however, the valve volume is increased and this contributes to the increase of dead volume of the pump.

It is possible to reduce the volume of a single valve by employing thin silicon wafers. Employing 350 μm thick wafers and keeping the nozzle opening fixed at 200 μm results in a reduction in volume of over 60%, as can be seen from the following table:

wafer th. (μm)	diffuser opening(μm)	valve volume (nl)	relative volume (%)
500	913	176.13	100.00
350	700	78.04	44.31
300	630	55.99	31.79

Table 1 Valve dead volume depending on wafer thickness

The minimisation of the valve number can negatively affect the maximum flow rate of the pump, so the designer has to exercise great care when deciding how many valves should be employed in the final pump design.

From simulations and previous experimental results [6], it was predicted that this pump would be operated between 3000 and 5000 Hz, hence designs with 3-5 valves have been considered in the design study presented here.

2.4 The piezo actuator

Chamber actuation results from lateral strain induced in the piezoelectric disk. One face of a piezoelectric disk is bonded to the chamber diaphragm (using an epoxy bonding layer); the other face of the disk is unconstrained. The piezoelectric disk is polarized in the axial direction, and each face is covered with an electrode.

Applying an axial electric field across the piezoelectric disk produces both a lateral and an axial response in the piezo-actuator, described by the d_{31} and d_{33} piezoelectric strain coefficients, respectively.

For this configuration, the chamber diaphragm bows to balance the lateral stress in the piezoelectric disk. Being clamped at the edges, the pump membrane is forced to move, or deflect, inward and outward, displacing a certain volume of fluid volume from and to the pump chamber. Therefore, it is of fundamental importance choosing an actuator material which offers the highest d_{31} strain coefficient.

Compared with the more commonly used Lead Zirconate Titanate (PZT) ceramics, <001> cut Lead Zinc Niobate Titanate (PZN-PT) single crystal exhibits higher piezoelectric coefficients; most importantly the d_{31} coefficient is almost 3 times as large as the PZT's (-1074e-12 C/N vs. -274e-12 C/N). It was anticipated in [9] that the use of a PZN instead of a PZT for a piezoactuator would yield a tenfold performance increases.

The actuator proposed here is made from PZN-PT piezo crystals, comes in "cut to spec" discs of fixed thickness as provided by TRS Ceramics, Inc.

3 MODELING OF MEMBRANE DEFLECTION AND VOLUME DISPLACEMENT

Since an analytical expression for the deflection is not readily available, numerical data were extracted from an FEM model.

3.1 Membrane deflection – ANSYS model

ANSYS 6.1 was used to simulate the mechanical behaviour of the pump membrane and the crystal actuator. The SOLID98 element was used to model the piezo material; while SOLID92, was chosen to model the Pyrex membrane.

The element sizes for the mesh were varied from 100µm to 200µm; appropriate boundary conditions were used to model the clamped edges and to exploit axial symmetry such that only one quarter of the membrane needed to be simulated.

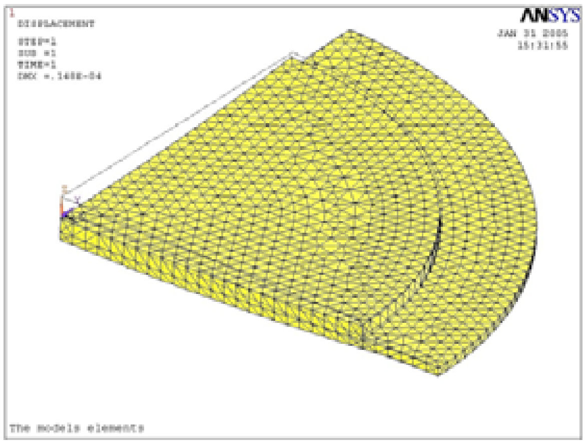

Figure 2 membrane and actuator deformed by an actuating voltage of 85V. Deflection profiles along a radial path have been collected for different ratios of actuator to membrane radius.

It was suggested in [4] that the optimum ratio of PZT to membrane radius was 0.8 which indeed yields the highest central deflection as shown in fig. 4. However, the shape of the displaced volume changes according to the ratio of radii, and fig. 3 suggests that values around 0.85 or higher could allow for a greater stroke volume of the pump.

3.2 Volume displacement model

The volume displacement was found by integrating the diaphragm deflection over the diaphragm area. The modelling methodology used is as follows:

1. All node coordinates and displacement data of the bottom membrane surface were exported from ANSYS into text files.
2. A C program reads and parses the text files and stores the data in Matlab array objects in a .mat – file.
3. A Matlab script reads the data set and linearly interpolates the deflection profile over a regular coordinate grid.
4. Two-dimensional integration in Matlab was performed over the interpolated data to obtain the volume enclosed by the deflected surface

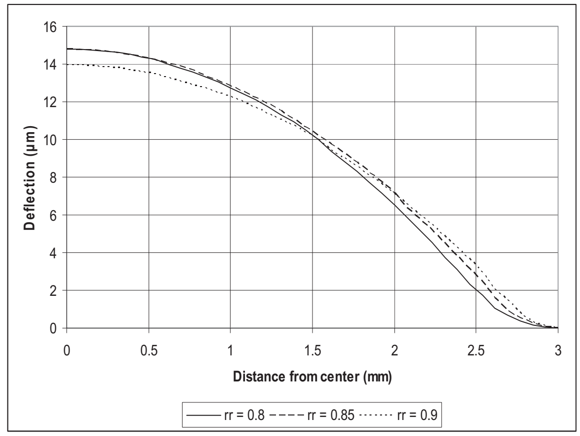

Figure 3 Deflection profiles for different radius ratios (0.8, 0.85, 0.9) simulated for a membrane thickness of 60 µm, PZN thickness of 100 µm and 85 V actuating voltage

From fig.3 it can be seen that the maxima for central deflection and displaced volume occur for different ratios: the highest deflection is achieved for 0.8; however the displaced volume is even greater for values between 0.85 and 0.9. That is because to a certain point, a larger ratio produces a flatter deflection profile, hence yielding a larger volume displacement and it is the displaced volume rather than the central deflection that determines the performance of a micropump.

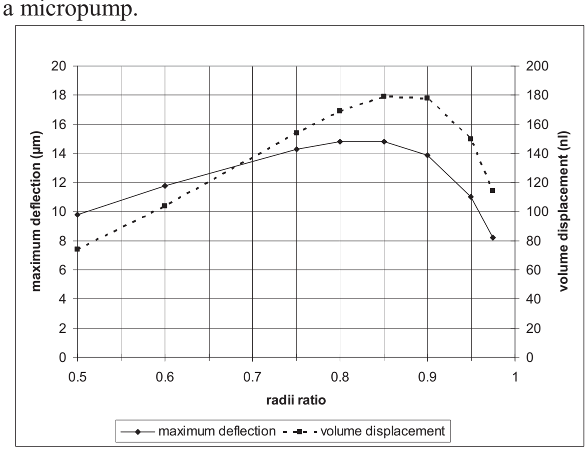

Figure 4 Maximum membrane deflection and volumetric displacement vs. PZN/membrane ratio

3.3 Actuator and membrane geometries

To further investigate the importance of the geometry of the membrane/actuator system, the shape of these elements has been varied as well. Micropump designs reported in the literature have used membranes and actuators of a square outline [5] because this can reduce cost and fabrication complexity.

A square membrane with a circular actuator and a fully square design have been simulated for various ratios of radii as well, referring to the 'radius' of a square as half of its side length. The volumetric displacement values obtained from the ANSYS simulations and Matlab integration are shown in figure 5. It can be seen that the fully square design can even achieve the same level of displaced volume as the fully circular one, but for a lower radius ratio of 0.75. The combination of square membrane and circular actuator, however, yields the highest volumetric displacement of all three configurations.

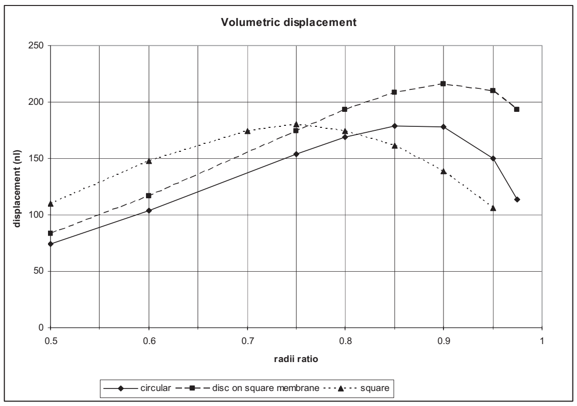

Figure 5 Volumetric displacement vs. PZN/membrane ratio for different membrane/actuator geometries: circular|circular, square|circular, square|square

This can be explained as follows: a circular actuator is optimally adapted to the deflection profile which has circular symmetry and a square membrane contains more elastic material to bend than a circular one.

It's important to characterize the maximum elastic stress that the deflection causes in the membrane. Borosilicate glasses have a maximum tolerable stress of at least 120 MPa which must not be reached during micropump operation. The maximum values of Von Mises stress for each of the ANSYS simulations have been plotted in figure 6. The fully square design creates a high level of stress which occurs in the corners of the actuator and is likely to damage the membrane material. The two circular actuator designs exhibit the same low stress for radii ratios up to 0.9 which is the interesting range. Given this observation and the high volumetric displacement, a square membrane with circular actuator at a radius ratio of 0.9 emerges as the optimal design choice for the micropump in question.

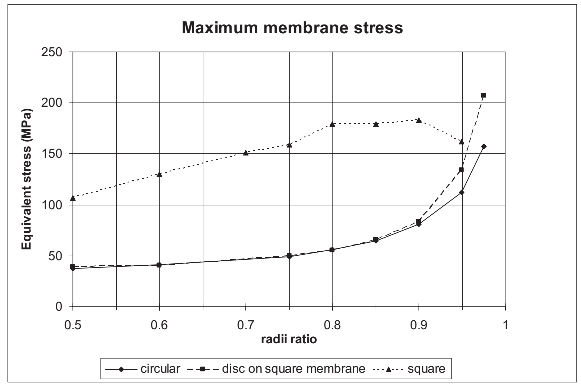

Figure 6 Equivalent stress vs. PZN/membrane ratio for different membrane/actuator geometries

4 CONCLUSIONS

We have shown that maximum membrane deflection for piezoelectrically actuated micropumps does not necessarily equal maximum volumetric displacement, thus a pump can be optimized for maximum flow rate better than previously thought possible.

We have demonstrated by means of FEM analysis that a square membrane with circular actuator at a radius ratio of 0.9 emerges as the optimal design.

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