Advanced SOI semiconductor structures for micro-dose biological samples handling

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The micro and nano-fluidics represents a milestone in the actual engineering and research area. Therefore the conceptual study of the structures by simulations is an important stage in design. The classical pumps with movable valves suffer from the fatigue of the movable parts, having a reduced lifetime and destroying some biological macromolecules. A valve-less micropump with a SOI membrane and a diffuser/nozzle element is in agreement with the silicon technology, being necessary special etching processes. This work proposes a micropump integrated in a SOI structure, dedicated to the bio-substances handling, as micro-dose of liquids. The simulations revealed the silicon membrane actuation, besides to the fluid flow through the valves. In this way, a designing method aided by simulations, was established as a further original issue of this paper.

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1. Introduction

A variety of chemical and biological procedures need tools that accurately deliver metered quantities of liquids [1]. New apparatus involved in the medical tests uses so called dry chemistry, with micro-liter of biofluids (e.g. 38÷250 µl in Spot-chem biochemical measurements), solid phase reagent and extreme low residues to avoid the environment contamination [2]. In this scope, some dedicated instruments must be developed: micropump, micropipettes for bioliquids delivery [3], microprobes or microgrippers for the cellular analysis [4]. In the microfluidics domain the micropump are used to transfer low quantities of fluids from an inlet to an outlet. Frequently, this situation occurs in the biological samples handling. Examples are offered in lab-on-chip, or in proteomics installation that must be able to handle up to 250 µl of human plasma per cycle [5]. In a previous work, a technological study presented a micropump for electrophoresis, inspired from SOI structures [6].

This paper is focused on the computer aided simulations of a valve-less micropump for biological usage. The implementation of this microstructure, using the advantages offered by the SOI (Silicon on Insulator) techniques, represent the original point of this paper. In fact, the proposed structure belongs to the Micro-Electro-Mechanical-Systems (MEMS). The possibility of the integration in a single chip of the mechanical actuator within an adjacent electronics, using the microtechnologies, stands for these devices as a strong interdisciplinary class.

The SOI structures generally offer some advantages in MEMS configurations. From the technological point of view, the buried oxide represents an excellent etching stop layer to prepare the upper membrane with an accurate thickness [7]. From the electrical point of view, the buried insulator completely avoids leakage currents from the electronic devices integrated onto the membrane toward substrate and consequently make impossible short-circuits with the biofluids beneath membrane. This paper proposes an additional facility offered by SOI architecture: two command gates - Front-Gate (FG) and Back-Gate (BG). The variable voltage applied over these gates, V_{F-B} , ensures the up and down membrane bending, so that the actuator is integrated inside the pump body.

This paper offers also a numerical study regarding the liquid flow through the diffuser/nozzle ducts and the mechanical stress in the etched membrane.

2. The SOI structure and materials

The entire SOI-MEMS system proposed in this paper is presented in Fig. 1. The actuator consists in a PZT layer deposited onto the Si-membrane that acts as a special insulator in the gate space of a SOI-MOSFET [8]. This piezo-layer is biased with two electrodes placed as Front-Gate and Back-Gate in order to achieve the reverse piezoelectric effect. The membrane represents the electronic device body for actuator. It is used only the capacitive parts from the SOI-MOSFET transistor in order to actuate the membrane. The Back-gate metallization reaches up to the Si-substrate, as is frequently used in the SOI devices [9]. In this way the membrane is up and down bending when a sinusoidal voltage is varying from -V_{F-B} to +V_{F-B.} Thus, the liquid flows from the input chamber into the pump chamber and then gets out thru the outlet, under the V_{F-B} control.

When the Si-membrane is down-bending, at $V_{F-B}>0$, the chamber volume decreases ("the pump mode") and the outlet duct acts as a diffuser with a lower flow restriction than the inlet duct, which play the nozzle role. A larger volume of liquid is transported out of the chamber through outlet than through input.



Fig. 1. The proposed SOI-MEMS structure.

When the membrane becomes up-bending, at $V_{F:B} < 0$, the chamber volume increases ("the supply mode") because a larger volume is transported into the chamber through the inlet duct that acts as a diffuser, than through the outlet duct that acts as a nozzle.

The V_{F-B} amplitude must ensure a maximum efficiency of the fluid transportation, but far away from the mechanical failure conditions.

Selecting others piezoelectric materials with better piezo-electric parameters (e.g. PXE5 instead of PZT), a better yield is achieved.

Additionally to the advantages mentioned in the introduction section, this structure has the following benefits: (a) it is working at a higher operation temperature as a conventional bulk Si device (from 120 °C for classical junction devices up to 300 °C for SOI devices), (b) doesn't suffer from the fatigue of some movable valves usually encountered in micropumps, (c) it is suitable for bio-liquids handling that can contain macro-molecules / cells, which can be damaged during the fluid transport by movable valves.

3. Membrane simulations

In the simulations, the sizes were selected accordingly with the biofluid delivery purpose. The mechanical stress in the SOI square membrane is simulated by Coventor in order to estimate the Si-film bending and to be sure that the mechanical failure will not appear. The following sizes 10000 μ m × 10000 μ m were selected for the square membrane. The classical SOI wafers offer different Si-film thicknesses from 0.2 μ m up to 10 μ m and thin BOX (Buried OXide), less than 1 μ m [10]. In simulations the thicknesses were: 0.6 μ m for Si-film and 0.4 μ m for BOX. Over the Si-membrane a PZT layer with dimensions 6000 μ m × 6000 μ m and 1 μ m thickness was deposited in simulations. The actuation voltage, V_{F-B}, was varied in the range 1V ÷ 20 V. The membrane deflection is observed, from simulations, in Fig. 2.



Fig. 2. Graph of the membrane deflection versus horizontal coordinate for positive V_{F-B} from 1V to 20V.

The maximum stress in the membrane is 4.5 MPa, at a potential drop of +20 V over PZT, far away from the strength limit – 30 MPa, but unsafe; the membrane displacement was 0.97 μ m. Also 20 V is a dangerous voltage from electrical point of view, due to the oxide breakdown by tunneling. Hence, the actuation voltage was reduced up to +5V, with 0.22 μ m displacement, Fig. 3.



Fig. 3.Cross-section through the Si-membrane / PZT for $V_{F-B} = 5V$.



Fig. 4. The mechanical stress in MPa, in the Si-membrane, actuated by the piezoelectric layer biased at 5V.

In Coventor, the input stimulus was the electrical signal (+5V) and the output functions were: the deflection and mechanical stress. The maximum mechanical stress,

 S_{xy} , developed in the horizontal plane xOy, reaches 0.52 MPa, safer for the failure conditions that occur in silicon, Fig. 4.

4. Valves simulation

The previous paragraph established the membrane displacements, $d_{1,2}$ respectively for down and up deviation of the membrane, at a given actuation voltage. From this displacement results the liquid volume variation into the pump chamber per cycle, V_c , and consequently the pressure applied on the diffuser / nozzle ducts, assimilated as valves. The liquid flow can be analytical studied by Bernoulli's law, or more accurately by Coventor microfluidics simulations.

Both ducts have the same shapes and sizes: pyramid-trunk with $l = 100 \mu m$, $L = 736 \mu m$, $H = 450 \mu m$, where l is the small base length, L is the big base length and H is the height. The pressure difference applied on the ducts was the same, but the flow sense was opposite for diffuser and nozzle. The diffuser is an expanding duct and the nozzle is a converging duct, both characterized by its specific pressure-loss coefficients $\zeta_{n,d}$. The pressure-loss coefficients are depending on the diffuser/nozzle geometry (l, L, H) and the velocities thru the throats [11].

Fig. 5 presents the velocity magnitude of the liquid particles in the diffuser valve with the vector representation. From these simulation results can be estimated the particles velocities thru the narrowest diffuser duct.



Fig. 5. The fluid velocity along the diffuser, with the vectors representation; velocity is expressed in µm/s.

Fig. 6 a, b offers the simulation result concerning the fluid pressure distribution inside the diffuser, respectively the nozzle, when a potential drop over the piezoelectric layer is +1V, that is equivalent with a maximum membrane deflection of 48 nm.

Fig. 6 proves that the pressure loss in the diffuser case reaches the maximum values 5.1 kPa in the smallest duct section, while in the nozzle smallest section the pressure reaches 0.062 kPa. This means that 98.78% from the maximum pressure exerts on the diffuser walls and only 1.22% exerts on the nozzle walls, suggesting a high yield for this pump without movable and tight valves.



Fig. 6. The pressure distribution in MPa: (a) The diffuser case; (b) The nozzle case.

5. Discussion

From the simulation results and the relationship among the pressure-loss coefficients and membrane size, the volume variation, V_c , of the pump chamber during a complete cycle is, [11]:

$$V_{c} = \frac{\pi D^{2}}{2} \cdot \left(d_{1} + d_{2} + \frac{d_{1}^{3} + d_{2}^{3}}{D^{2}} \right) \cdot \frac{\sqrt{\zeta_{n}/\zeta_{d}} - 1}{\sqrt{\zeta_{n}/\zeta_{d}} + 1} \quad (1)$$

where $d_{1,2}$ are the vertical deviations, D is the membrane length. For the above sizes, the pressure loss coefficients are estimated to be: $\zeta_d=0.96$, $\zeta_n=1.94$.

Finally, the net flow-rate can be computed as a global parameter, establishing a period-time for the variable actuating voltage. In our case, from Fig. 3 results $d_1=d_2=0.21 \ \mu m$ for $V_{F-B}=\pm 5V$ and the chamber volume variation results from eq. (1): $V_c=13 \times 10^{-3} \mu l$ per cycle.

From the microfluidics simulations, like Fig. 6.a.b, the flow-rate is extracted as 50.5 μ l/s for diffuser and as 26.7 μ l/s for nozzle. Hence, the net flow-rate is 23.8 μ l/s for the micropump actuated at V_{F-B}=±1V.

Similarly, for $V_{F-B}=\pm 5$ V the net flow-rate is 46.4 µl/s. Taking into account that $V_c=13$ nl/cycle for $V_{F-B}=\pm 5$ V, the period of the AC signal results: $T=V_c/Q_v=0.282$ ms and the frequency f=1/T=3.5 kHz.

These net-flow rates are suitable for biomedical applications, with liquids quantities about 10...250 μ l. The micropump parameters are also in agreement with the data from literature [12]. A similar valve-less micropump with diffuser/nozzle ducts and a silicon rubber membrane with 2 mm width was reported. It was stimulated at minimum 6.9 V in order to provide a deflection of 0.76 μ m. Applying a variable voltage with 0.540 kHz on an actuator, the net flow-rate for water was 0.05 ml/min = 0.8 μ l/s [12], so lower than that obtained in the presented SOI structure.

6. Conclusions

This paper investigated a global behavior of a SOI-MEMS structure working as a micropump for small quantities of liquid delivering, suitable in the bio-medical applications. The simulator was able to receive as input signals some variable voltages, applied between a Front and a Back gate, to model the reverse piezoelectric effect in the PZT layer integrated onto the upper SOI membrane and to convert the voltage in a membrane deflection. By simulations were checked the failure conditions. Increasing the actuation voltage, a higher deflection of the membrane is produced with a better net-flow, besides to a higher power consumption.

Hence, the maximum voltage accepted for actuation was ± 5 V. The simulations of the liquid flow through the diffuser-nozzle ducts make possible the net flow-rate extracting: 23.8 µl/s up to 46.4 µl/s for the incident stimulus ranging from +1V up to 5 V.

As actuating element, the SOI membrane covered by a PZT material presents higher performances versus the traditional rubber membrane and a technological compatibility among etching processes in Si. The diffuser and nozzle valves have the advantage to not destry some macromolecule from the biological samples.

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