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DESIGN AND SIMULATION OF AN OPTICAL MICROSENSOR FOR MEASURING PRESSURE IN BIOLOGICAL FLUIDS

Braggio Luciano[a] **and Guarnieri F. Ariel**[a,b]

[a]*Universidad Nacional de Entre Ríos – Facultad de Ingeniería – Carrera de Bioingeniería*
http://www.bioingenieria.edu.ar

[b]*Centro Internacional de Métodos Computacionales en Ingeniería (CIMEC), Instituto de Desarrollo Tecnológico para la Industria Química (INTEC), CONICET*
Email: luciano.braggio@gmail.com

Abstract. Aim:To develop an opto-mechanical FEM model for monitoring local pressure in microfluidic devices using a deformable diffraction grating. Material and Methods: A FEM mechanical model is developed using 2D solid elements to calculate the deformation of the gratings on an elastomeric diaphragm subjected to a fluid pressure. The deformed geometry is exported to an optical software for diffraction analysis. A moulded PDMS chip with a grating consisting of 1μm wide, 1 μm deep rectangular grooves arrayed with a period of 2μm is mechanically simulated for validation. The deformed geometry is obtained after applying an internal pressure. The optical response of the device to a varying pressure is presented and compared with the theoretical prediction.

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1 INTRODUCTION

Biomedical and biological areas are highlighted as new application areas of MEMS technology. The micro-opto-electro-mechanical systems (MOEMS) have become popular as they can be used in microscale applications which may need optical elements. They can also be combined with other microsystems. Several different types of MOEMS are being used for monitoring local pressure, especially in the area of microfluidics (Yu and Zhao, 2009; Chronis et al., 2003; Yoon et al., 2010; Cao et al., 2011; Hosokawa and Maeda, 2001; Rogers et al., 1996).

A repetitive array of diffracting elements, either apertures or obstacles that has the effect of producing periodic alterations in the phase, amplitude, or both of an emergent wave it is said to be a diffraction grating. When the regular variations in the thickness of the surface yield a modulation in phase, we call this type of grating a phase diffraction grating. Moreover, if we have a reflective surface we call this a reflection phase grating, as shown in figure 1. Microfluidic diffraction gratings might serve as sensing elements in micro total analysis systems (mTAS) where the dimensions of the gratings are compatible with the microfluidic devices (Schueller et al., 1999).

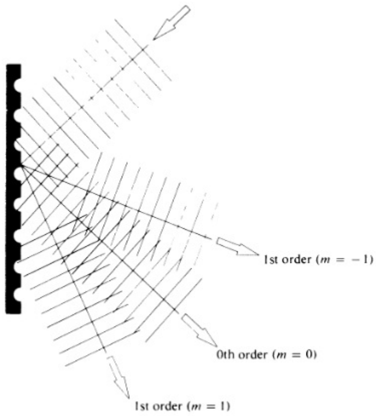

Figure 1: Reflection phase grating

Poly (di-methyl-siloxane)(PDMS) has proven to be an excellent material for micro- and nanotechnologies (Hosokawa and Maeda, 2001). PDMS can be deformed reversibly and repeatedly without residual distortions and is thermally stable, inexpensive (Qin et al., 1998), nontoxic and commercially available. Values of Young's modulus for PDMS have been reported from around 0,35 to 3 [MPa](Foland et al., 2011). Micro-devices made from PDMS are easy to fabricate using the replica moulding technique (Qin et al., 1998). There have been several works reporting on PDMS MOEMS with different applications and physical principles such as guided-mode resonance (GMR), angular deviations of the diffracted beams, and changes in reflectivity among others (Yu and Zhao, 2009; Chronis et al., 2003; Cao et al., 2011; Hosokawa and Maeda, 2001). PDMS has many features which makes it an excellent material for a pressure sensor, e.g. good biocompatibility, nontoxic and optically transparent (Chronis et al., 2003), easily fabricated and widely used in micro-fluidic devices (Yu and Zhao, 2009). PDMS might be used as a biomedical material due to its excellent aspects like microfabricability, biocompatibility, and robust

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functionality. The major advantages of PDMS can be found in its fabrication process and material properties. The PDMS microfabrication, generally called soft lithography, is relatively easy. Many inexpensive parts from the same mold can be produced and miniaturized structures of submicrometer size can be achieved. Moreover, PDMS offers transparency in the ultraviolet and visible spectral. It is chemically inert, except to nonpolar solvents, and finally, it has a relatively low elastic modulus (Yoon et al., 2010).

In this paper we describe the simulation and performance of a passive pressure sensor based on an elastomeric diffraction grating. We develop an opto-mechanical model for monitoring local pressure in microfluidic devices. A coupling between a mechanical FEM model and an optical model based on ray tracing technique is made.

2 MATERIALS AND METHODS

2.1 DEVICE CHARACTERISTICS AND OPERATING PRINCIPLE

The device consists of a binary phase surface-relief grating on a millimeter-thick section of PDMS. The diaphragm has a circular shape with a radius of 5[mm] and a thickness of 25 [um]. The operating principle of the detector is that a deflection of the PDMS membrane is induced by the pressure applied on the opposite face of the diaphragm. As the pitch of the diffraction grating varies, it causes a shift in the angular positions of light beams deviated from the optical sensor.

As it was said above, the PDMS is optically transparent to visible light. Therefore, a thin coating of a reflective material is needed in order to reflect it.

2.2 THEORY

2.2.1 Mechanical Model

A finite element analysis software was also used to simulate the mechanical deformation of the membrane under uniform pressure

Finite element simulations were performed to visualize the cross sectional view of the membrane and to determine its curvature radio. The main purpose of the mechanical simulation was to analyze the pitch variation of the grating and the curvature of the membrane, in order to use this data as input parameters in the optical model.

In the computational analysis, PDMS is assumed to have a density of 0.971 kg/m3 and a Poisson's ratio of 0.48, which is used to prevent a numerical error in calculation, although the published one is 0.5 (Yoon et al., 2010). The thickness and Young's modulus of the PDMS membrane were assumed to be 25 microns and 3 [MPa] respectively.

A simplified theoretical model for the PDMS membrane is derived on the basis of the following assumptions:

1. The membrane is assumed to be flat with no pressure, of uniform thickness, and of homogeneous isotropic material.

2. The thickness of the sensor is less than one-tenth of the diameter, which means that it is a thin membrane.

3. The applied pressure is always normal to the surface of the membrane.

4. The deformed surface under pressure is assumed to remain spherical with uniform thickness throughout deformation.

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5. As mentioned below, the diffraction grating is a reflective one; consequently, because PDMS is transparent to the visible spectrum of light we must deposit a fine coating of a reflective surface. This coating is not considered in the simulation, as it has a thickness in the hundreds of nanometers.

A linear elastic model was used to simulate the mechanical behavior of the PDMS membrane, considering an axial symmetry situation, where cylindrical coordinates are used. The simulation model solves equations for the global displacement in the r and z directions and the strains. Because of the axial-symmetric assumption, any of the stresses and strains involving the azymuthal component are zero. Loads are independent of φ and loads only in the r and z directions are permitted. A 3D static analysis was also performed, in order to have a qualitative idea of the grating´s pitch deformation. We considered a large-displacement analysis, i.e. the deformations were not small and the strains were calculated without restrictions. The resulting strains are known as Green or Green-Lagrange strains, and large displacement is sometimes referred to as geometric nonlinearity or nonlinear geometry. There are no initial, neither thermal stresses in the model.

The symmetric strain tensor ε consists of both normal and shear strain components:

$$\varepsilon = \begin{pmatrix} \varepsilon_x & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{xy} & \varepsilon_y & \varepsilon_{yz} \\ \varepsilon_{xz} & \varepsilon_{yz} & \varepsilon_z \end{pmatrix} \tag{1}$$

For the axial symmetry case, the relationships between the strains and displacements are

$$\varepsilon_r = \frac{\partial u}{\partial r} \quad \varepsilon_\varphi = \frac{u}{r} \quad \varepsilon_z = \frac{\partial w}{\partial z} \quad \gamma_{rz} = \frac{\partial u}{\partial z} + \frac{\partial w}{\partial r} \tag{2}$$

The Green strain components ε_{ij} are

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} + \frac{\partial u_k}{\partial x_i}.\frac{\partial u_k}{\partial x_j}\right) \tag{3}$$

The path that a physical particle describes as it is subjected to deformation is described by equation 4. Both the deformed and undeformed positions were measured in the same coordinate system. Using the displacement u, it is then possible to write equation 5. The deformation gradient F is defined by equation 6.

$$\mathbf{x} = \mathbf{x}\left(\mathbf{X},t\right) \tag{4}$$

$$\mathbf{x} = \mathbf{X} + \mathbf{u} \tag{5}$$

$$d\mathbf{x} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}} d\mathbf{X} = \mathbf{F} d\mathbf{X} \tag{6}$$

As mentioned above, the membrane with the diffraction grating is made of PDMS. Therefore, we consider PDMS as an linear elastic material and the governing constitutive equation, under the assumptions already expressed, is

$$\sigma = D\varepsilon_{el} \tag{7}$$

where D is the elasticity matrix and ε_{el} is the strain given in vector form. The PDMS in the simulation was treated as an isotropic material.

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GEOMETRY OF THE MODEL The PDMS membrane is 10.0 mm in diameter and 25 [um] thick. In this situation, the membrane would deform due to the applied pressure.

BOUNDARY CONDITIONS The assumptions made in the model, as shown in figure 2, are:

1. Axial symmetry: this is the revolution axis.
2. Applied pressure: in the opposite direction of the surface normal-vector.
3. Free boundary-condition: the rest of the geometry, except the edge of the membrane.
4. The edge of the membrane (not shown in the figure) is fixed.

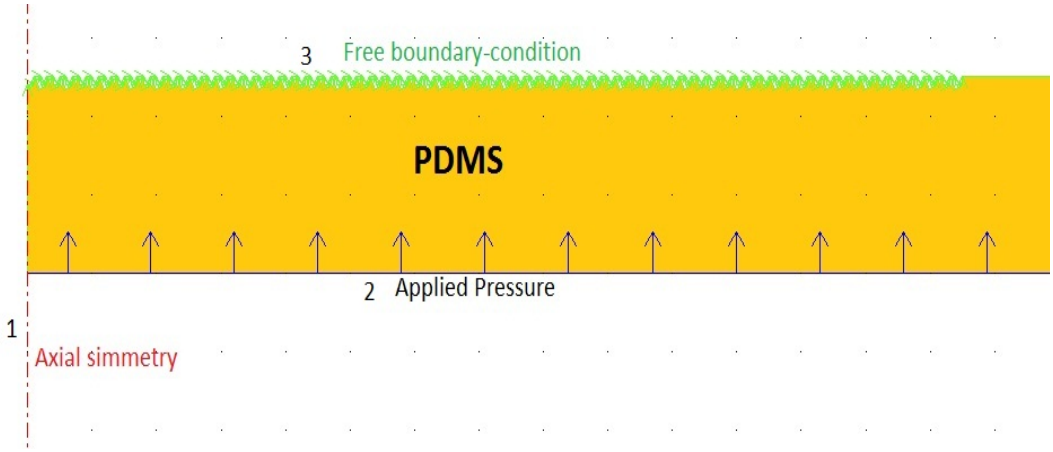

Figure 2: Boundary conditions of the mechanical model

MESH, TYPE AND NUMBER OF ELEMENTS The mesh consisted of 8976 triangular-shaped elements. The type of element used was a Lagrange-quadratic.

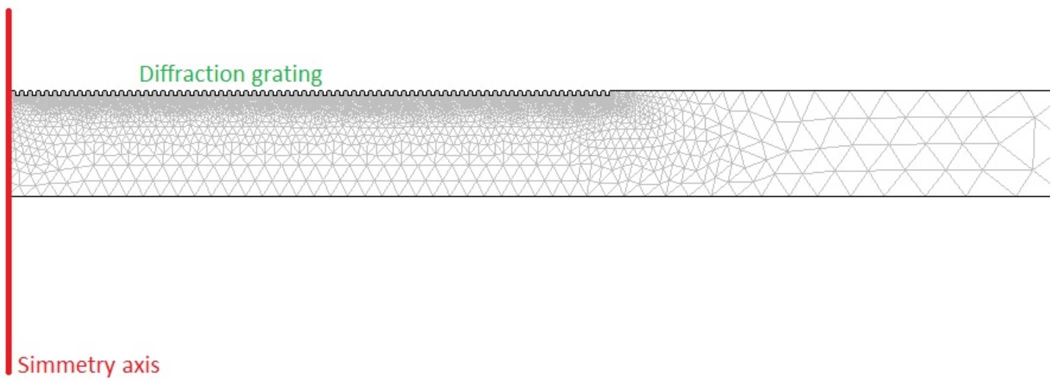

Figure 3: Meshed geometry with zoom at the grating area

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SOLVER Both a static and a parametric analysis were performed. In the first instance, the pressure was set at the value of 2000 [Pa]. In the parametric analysis the pressure ranged from 0 to 2400[Pa] in order to determine the measuring range of the sensor and its sensitivity.

The solver used was the UMFPACK solver. For the parametric analysis the time of computing was 241,897[s] in a dual-core machine. The number of degrees of freedom solved for was 43445.

OPTICAL MODEL With the results obtained from the mechanical simulation, the curvature radius of the diaphragm was determined. The most important reason for performing the mechanical simulation of the PDMS diffraction grating was to obtain the pitch variation as the membrane deformed due to the applied pressure. This is the operating principle of the opto-mechanic passive sensor.

In order to measure the value of the pressure acting on the membrane, the angular deviation of the light spots was analyzed. The diffraction grating acts deviating each spectral component of the light in different angles. For a given expansion, the highest-order diffracted beams generated by probing at large angles of incidence underwent the largest angular deflections. Light diffracted from a grating appears in angular locations determined by

$$\sin(\theta) - \sin(\theta_0) = \frac{m\lambda}{d} \tag{8}$$

where θ is the angle of diffraction for the mth-order beam, θ_0 is angle of incidence of the probing beam, λ is the wavelength of the probing light, and d is the pitch of the diffraction grating. The pitch of the diffraction grating is the distance between any two consecutive grooves from the grating. As the diaphragm is deformed because of the pressure being applied, the pitch varies, i.e. the optical behavior of the sensor changes. This change in the pitch is proportional to the applied pressure. Hence, we can measure the value of the pressure from the angular deviations of the light spots.

In the optical analysis, the wavelength range simulated was the visible spectrum. This was made in order to get an understanding of the angular deviation that each wavelength suffers and to estimate the spectral resolution of the diffraction grating. The detection was performed with a plane detector surface, which measures the irradiance in each of the pixels comprising the detector, e.g. like a CCD sensor of a camera, in order to determine the position of the spot of lights and the correlation with pressure.

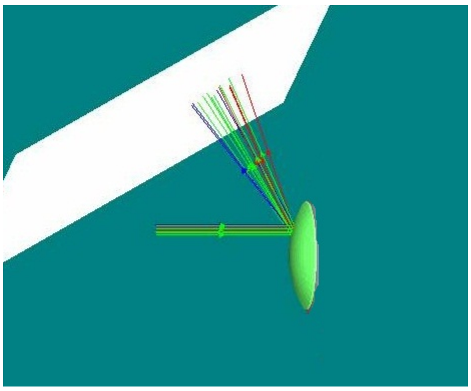

Figure 4: Diffraction of the incident beam.

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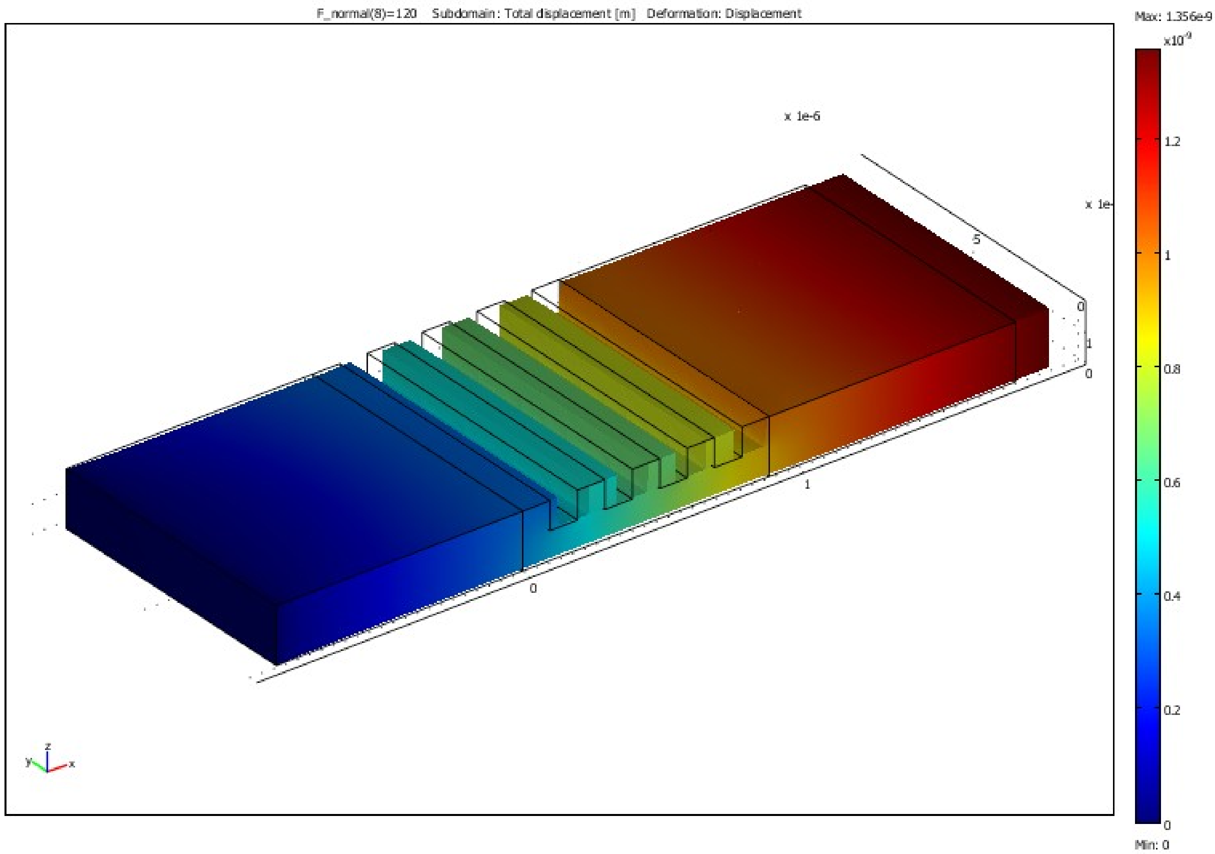

Figure 5: Deformation of the diffraction grating.

3 RESULTS AND DISCUSSION

3.1 Results

Two principal sets of simulations and analyses were carried out to evaluate the behavior of the PDMS pressure sensor. First, the mechanical properties of the diaphragm were simulated with a Finite Elements Analysis. In figure 5 it is shown how the pitch of the diffraction grating is subjected to a deformation and varies its pitch. A force on the side of the membrane is exerted in order to check the variation in the pitch.

Deformation and vertical displacement of the membrane Displacement of the apex of the membrane at maximum applied pressure was evaluated in order to calculate the major pitch variation from the initial value. Figure 6 shows the vertical (z-component) displacement of the membrane when a pressure of 2400[Pa] is applied. Next, the radius of curvature was computed taking information of the coordinates of three points of the diaphragm. Figure 7 describes the displacement of the apex from its initial value as the pressure is increased.

Analyses of the optical properties Once the updated pitch value was derived from the mechanical model, these data were entered as parameters of the diffraction grating in the optical model. In figure 8 it is shown how different sectors for targeting the incident light were con-

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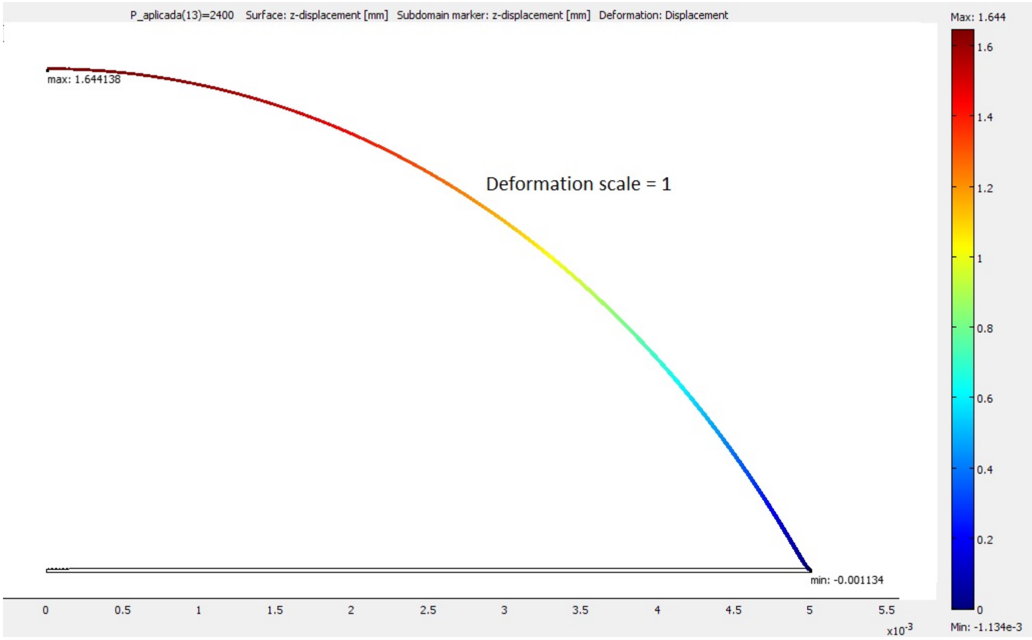

Figure 6: Displacement and deformtion of the membrane when pressure is applied.

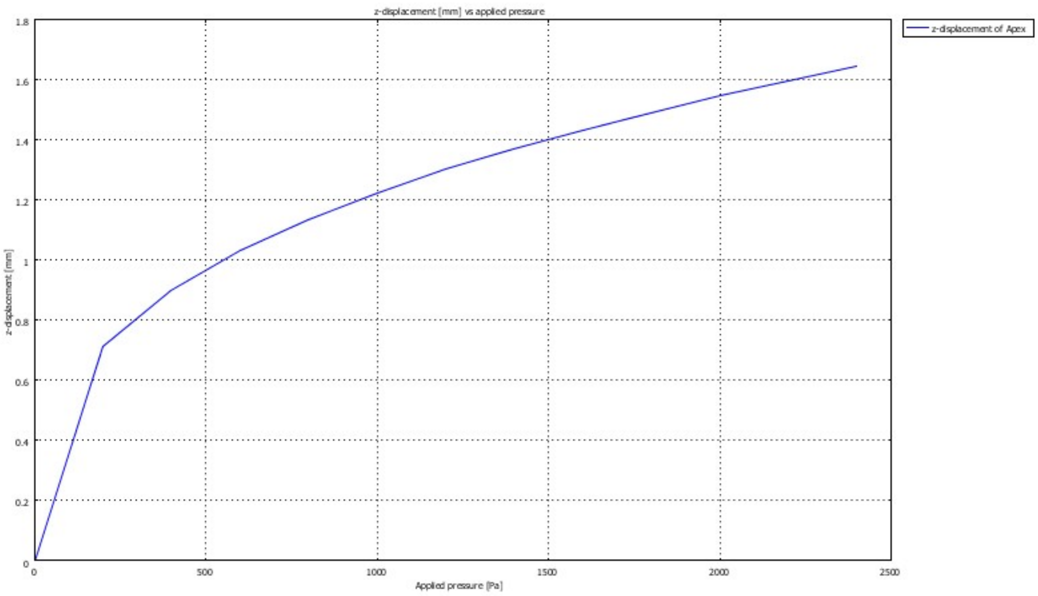

Figure 7: Vertical displacement of the apex as the pressure ranges from 0 to 2400 [Pa]

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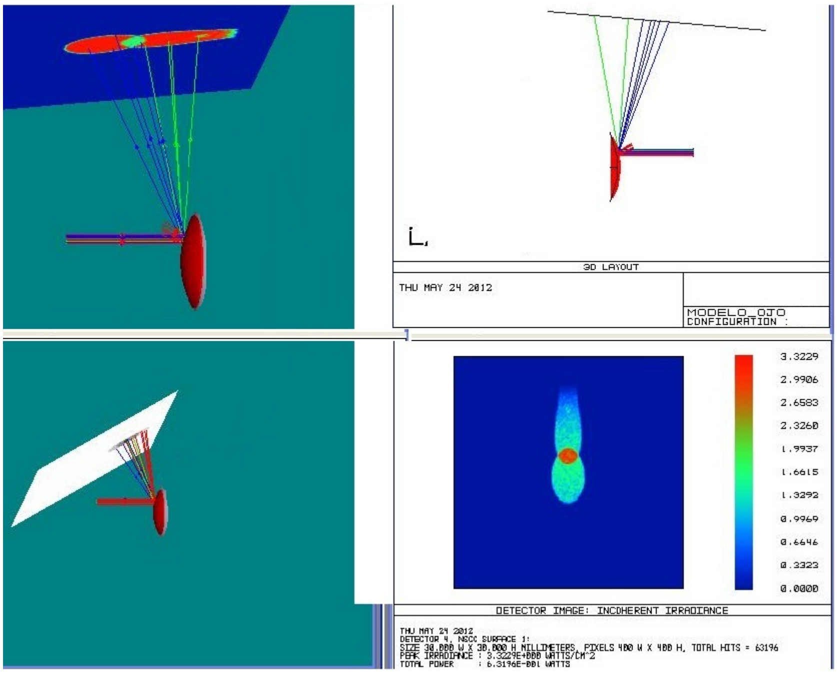

Figure 8: Schematic diagram of the optical sensor at differents detector-positions.

sidered. The spectral resolution of the grating and the best position of the detection plane were also studied.

Figure 9 plots the angular deflections in the first-order spots of the probing beam when polychromatic light (486[nm]; 587[nm]; 656[nm] the F, d, C spectral lines) was directed into the sensor. The sensitivity to changes in the radius of curvature was considered. Because the probing beam was aimed at the center of the membrane (the apex), there were no considerable variations in the position of the diffracted beams. It is also shown that for each wavelength (denoted by 1, 2 and 3) the change in the positions of the spots (denoted by 1', 2' and 3') when the maximum pressure of 2400[Pa] was applied. The remaining spots in the figure correspond to different radius of curvature as mentioned above.

4 CONCLUSIONS

A pressure sensor based on PDMS diffraction grating was simulated. An opto-mechanical model was used in the pressure range of interest and resulted in a shift in the angular positions of light beams diffracted from the grating. From the analyses made, pitch variation was demonstrated. The sensitivity to changes in the radius of curvature was considered. Because the probing beam was aimed at the center of the membrane, there were no considerable variations in the position of the diffracted beams. The variations in the pitch due to mechanical deformation produced sufficient optical response to applied pressure ranging from 0 to 2500[Pa].

The PDMS deformable diffraction grating showed to be useful for monitoring local pressure.

5 ACKNOWLEDGEMENTS

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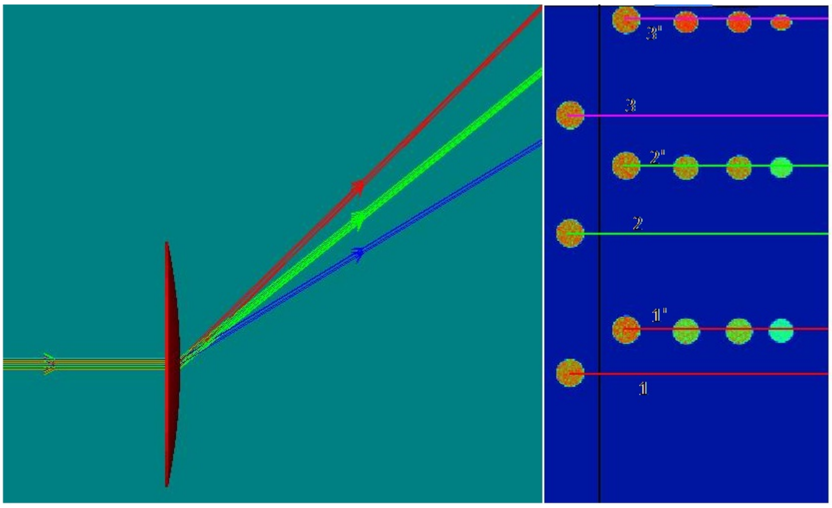

Figure 9: Deviation of the diffracted spots as the pitch varies.

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