High sensitivity piezoresistive cantilever sensor for biomolecular detection

Johnny H. HE* and Yong Feng LI
Institute of Microelectronics, 11 Science Park Road, Singapore 117685

*Contact Email : han@ime.a-star.edu.sg

Abstract. Micro-cantilevers are now gaining popularity in biomolecular sensing. Monitoring and mass detection of biological species can be accurately determined using the micro- or nano- scale cantilevers. The targeted biological molecules are first immobilized onto the micro-cantilever which is later determined through static or dynamic techniques. Optical detection method is employed to determine the deflection of the cantilever in static analysis or the shift of resonance frequency in dynamic analysis. Though both analyses using optical detection have been highly sensitive and produce accurate results, they required extensive and expensive experimental setup and are not practical for point-of-care application. Piezoresistive sensing has become an alternative approach in biological sensing as changes in mechanical properties can be converted to electrical output. This paper presents the design and simulation of a highly sensitivity piezoresistive based micro-cantilever for biomolecular detection. A series of holes are formed on the silicon based micro-cantilever. These discontinuities form the Stress Concentration Region (SCR) used to increase sensitivity for piezoresistive sensing. Finite Element Analysis (FEA) through ANSYS 8.0 was performed on the structural model to maximize the SCR so as to improve the sensitivity of the cantilever. The optimized number, geometry, radius, and the distance from the first hole to the root of these holes were discussed in this paper.

1. Introduction
Micromachined cantilevers are gaining more and more interest as biochemical sensors, where the way in which the binding of chemical species changes the mechanical properties of the cantilever is utilized. These biological molecules are first immobilized onto the micro-cantilever which is later determined through static or dynamic techniques. In static detection, molecular binding onto the surface of a cantilever beam induces stress gradient across the thickness of the cantilever. This creates a bending moment on the ultra thin cantilever, where the optical methods can then be used to determine the deflection of the light beam[1],[2]. In the dynamic analysis, targeted species that bind onto the cantilever surface will produce a shift in resonance frequency of resonating structures[3],[4]. Both of the static deflection and the shift in resonance frequency can be measured via an optical laser readout scheme. However the optical readout system required is usually bulky and not portable. At the same time it requires accurate alignment of the laser spot onto the cantilever, which can be very time-consuming. An alternative approach to detect the signals is to use piezoresistive cantilever sensor in which the changes in mechanical properties are converted to electrical output[5].
Our objective is to optimize the sensitivity of the piezoresistive cantilever by the introduction of SCR. With the help of ANSYS 8.0 Finite Element Analysis simulation, we study the effect of different geometry, position and size of the Stress Concentration Region (SCR) on the value of the difference between longitudinal and transverse stress experienced by the cantilever beam. By doing so, a design that maximizes the surface stress difference is obtained. Hence the sensitivity is optimized.

2. Literature review
SCR is the result of discontinuities such as holes, grooves, keyways, cracks or sharp change in one of the dimensions of the structure. These structural discontinuities enhance the stress around their proximity.

Resistance change can be calculated using the following formula
\[ \frac{\Delta R}{R} = \sigma_l \pi_l + \sigma_t \pi_t. \]  
(1)

where \( \sigma_l \) and \( \sigma_t \) are the longitudinal and transverse stress components, \( \pi_l \) and \( \pi_t \) are the longitudinal and transverse piezoresistance coefficients. In <110> direction of P-type resistor, \( \pi_{44} \) is more dominant over the other two coefficients \( \pi_{11} \) and \( \pi_{12} \). Hence the above equation can be approximated by
\[ \frac{\Delta R}{R} = \frac{\pi_{44}(\sigma_l - \sigma_t)}{2}. \]  
(2)

From the above equation, we can see that the resistance change is increased by maximizing the differential stress \( (\sigma_l - \sigma_t) \).

The piezoresistive sensitivity, which is defined by the ratio of cantilever resistance change to the end deflection of the cantilever, is given by
\[ \frac{\Delta R}{R} \bigg/ \Delta z = \frac{-3\pi E t (1 - L/2)}{2l^3} = \frac{3K t (1 - L/2)}{2l^3}. \]  
(3)

where \( \Delta z \) is the vertical displacement of the cantilever end, \( \pi_l \) is the longitudinal piezoresistive coefficient, \( E \) is the Young modulus, \( K = \pi_l E \) is the gauge factor, \( l \) and \( t \) is the cantilever length and thickness and \( L \) is the piezoresistive doping length \([7]\).

A few groups have devoted their time to the enhancement of the surface stress. Ryu et al.\([8]\) concluded that shorter cantilever had higher sensitivity and the width of the cantilever did not have any effect on sensitivity. Furthermore the sensing area should be confined to the root of the cantilever. Rectangular holes on the cantilever aligned in the longitudinal direction were used as SCR by Kassenge et al.\([9]\) These holes increase the longitudinal stress much more than the transverse stress resulting in a higher \( (\sigma_l - \sigma_t) \) and in turn boost the sensitivity of the cantilever. Mo et al. have come out with an optimum design of C-shaped cantilever with elliptical holes on it\([10]\).

3. Design and simulation procedures
Below is a flowchart of the simulations performed. A rectangular cantilever, as shown in figure 1(a) and (b), is modeled using ANSYS, having length of 20\( \mu \)m, width of 3.2\( \mu \)m, thickness of 0.2\( \mu \)m. It is made of polysilicon, having Young’s modulus of 170GPa and Poisson’s ratio of 0.22. A pressure of 3.07Pa (equivalent to 10ng of mass) is applied on an area of 10\( *3.2\mu m^2 \) from the free tip.
First of all, the Average Stress Difference (ASD) around one hole of different shapes is calculated. ASD is defined as the ratio of the total differential stress ($\sigma_r - \sigma_t$) in a given volume to the volume itself. The volume is defined in a way such that it has a length equal to the diameter or the length of the hole plus 0.5μm from both sides of the hole, a width of 3.2μm and a thickness of 0.02μm, as shown in figure 3.1(c). The perpendicular distance from the root of the cantilever to the side of the hole, $D_h$, is all fixed to be 0.5μm. The polygonal holes are inscribed in a circle of radius 0.8μm. The circular hole has a radius of 0.8μm while the elliptical hole has a transverse diameter of 1.6μm and longitudinal diameter of 1μm. From ANSYS, the total elemental solution of stress difference of the defined volume can be obtained. Then the ASD can be calculated from total stress difference divided by the volume. The results are recorded in Table.1.

After the shape of hole that gives the highest ASD is found, the effect of adding more holes of this best shape is investigated using a similar ANSYS program. Again, the ASDs around the first hole are compared. The results are recorded in Table.2.

The next step is to determine the optimum position and size of the hole or holes of the best shape. In this case, $D_h$ for the position and the radius $r$ for the size are varied while we only use only one octagonal hole.

After all the above simulations are done, the width and the length of the cantilever are increased proportionally to two and three times respectively. This is to study the size effect on the differential surface stress, i.e. whether the stress go up when the cantilever gets bigger. At the same time we would like to determine if the same trend we obtained for a specific dimension of the cantilever will appear in other sets of dimensions.

4. Simulation results
Seven types of holes are simulated and the results are shown in Table.1. We can see that octagonal hole gives the highest value of ASD. The differential stress profile ($\sigma_r - \sigma_t$) of a cantilever with an octagonal hole is shown in figure 2. One possible explanation of octagonal hole giving the highest ASD may be that the sharp corners of the hole create SCRs. When we use a higher order of polygons,
there are more sharp angles and hence more SCRs around the hole. This will give rise to a higher value of ASD.

| Shape of the hole                | Average Stress Difference (MPa/μm³) |
|----------------------------------|-------------------------------------|
| Simple cantilever without any hole | 439                                 |
| Rectangular hole                 | 589                                 |
| Square hole                      | 563                                 |
| Hexagonal hole                   | 591                                 |
| Septagonal hole                  | 666                                 |
| Octagonal hole                   | 690                                 |
| Circular hole                    | 621                                 |
| Elliptical hole                  | 590                                 |

Figure 1(a) and (b) is the top and cross-sectional views of a cantilever with an octagonal hole. (c) shows the defined volume for calculation of the Average Stress Difference. It is a volume around the hole with length equal to the diameter of the hole plus 0.5μm from both sides of the hole, width of 3.2μm and thickness of 0.02μm.
Figure 2 shows the differential stress profile ($\sigma_l-\sigma_i$) of a cantilever with an octagonal hole

The effect of adding more octagonal holes to the cantilever is studied. Table 2 is the ASD around the first hole when different number of octagonal holes of same size is added along the length of the cantilever with the same spacing between the holes.

It shows that the addition of more holes to the cantilever does not help to enhance the ASD around the first hole which is nearest to the root of the cantilever. Hence one octagonal hole is enough to maximize the differential stress. This is probably due to SCR is a local effect where the addition of more holes does not help to increase the stress concentration near the first hole.

Table 2 ASD around the first hole when different number of octagonal holes is added to the cantilever

| no. of holes | Average Stress Difference (MPa/µm²) |
|--------------|------------------------------------|
| 1            | 689.7559                           |
| 2            | 686.4751                           |
| 3            | 686.8622                           |
| 4            | 686.9098                           |

After the optimal geometry and the number of hole are determined, the dimension and the position of the hole are investigated. Figure 3(a) shows that the larger the radius of the octagonal hole, $r$, the higher the differential stress around the first hole. Whereas (b) tells us the closer the hole to the root of the cantilever, the higher the differential stress. $D_h$ is defined as the distance from the root of the cantilever to the first hole.
Variation of $r$ of octagon

Average Stress Difference (MPa/um$^3$)

| 0  | 200 | 300 | 400 | 500 | 600 | 700 | 800 | 900 |
|----|-----|-----|-----|-----|-----|-----|-----|-----|
| 0  |     |     |     |     |     |     |     |     |
| 0.5|     |     |     |     |     |     |     |     |
| 1  |     |     |     |     |     |     |     |     |
| 1.5|     |     |     |     |     |     |     |     |

Variation of $D_h$

Average Stress Difference (MPa/um$^3$)

| 0  | 300 | 350 | 400 | 450 | 500 | 550 | 600 | 650 | 700 |
|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 0  |     |     |     |     |     |     |     |     |     |
| 1  |     |     |     |     |     |     |     |     |     |
| 2  |     |     |     |     |     |     |     |     |     |
| 3  |     |     |     |     |     |     |     |     |     |
| 4  |     |     |     |     |     |     |     |     |     |
| 5  |     |     |     |     |     |     |     |     |     |
| 6  |     |     |     |     |     |     |     |     |     |

Figure 3(a) Plot of ASD against the radius of the octagonal hole, $r$. It can be seen that the larger the radius the higher the differential stress around the first hole. (b) Plot of ASD against the distance from the root to the hole, $D_h$. The closer to the root, the higher the differential stress.

To get a more generalized picture of the effect of changes in the size and position of the hole on the ASD value, we perform another series of simulations. Previously we are investigating a cantilever beam of 20*3.2*0.02μm$^3$. Now we enlarge the model by making its length and the width of 2 times and 3 times larger, i.e. 40μm long, 6.4μm wide and 60μm long and 9.6μm wide while the thickness remains 0.2μm. $r$ and $D_h$ are increased accordingly so that the ratio of $r/w$ and $D_h/l$ remain constant throughout. The loading condition is the same for the series of the simulations. By using the same method of extracting ASD as in previous experiments, we have the results as shown in figure 4. The same trend is repeated regardless of the size of the beam -- (1) the larger the radius of the octagonal hole, $r$, the higher the differential stress around the first hole and (2) the closer the hole to the root of the cantilever, the higher the differential stress.

Figure 4(a) Plot of ASD against the ratio of $r/w$ and (b) Plot of ASD against the ratio of $D_h/l$ for different magnification of the cantilever beam. It can be seen that the same trend appears for different dimension of the cantilever -- the larger the radius and the closer to the hole to the root, the higher the differential stress around the first hole.

5. Conclusion

With the help of ANSYS simulation, the effect of different geometry, number, dimension and position of holes added to the cantilever, on the differential stress around the hole, has been studied. The design guidelines for a high sensitivity cantilever would be one octagonal hole positioned as close to the root as possible with its radius as large as possible. However, there are other factors to consider. For instance, if the hole is too large, the distance from the side of the hole to the side of the cantilever will be very small, inducing reliability problem of the cantilever, i.e. easy to fracture. Furthermore, it is difficult to do patterning in such a small space when we incorporate piezoresistive sensing into the
beam. The future work will be the follow-up study of implementing the piezoresistive doping in the SCR so as to produce a piezoresistive cantilever sensor with high sensitivity.

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