Design Issues in SOI-Based High-Sensitivity Piezoresistive Cantilever Devices

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ABSTRACT

In this work, the mechanical design and optimization of high-sensitivity piezoresistive cantilevers used for detecting changes in surface stresses due to binding and hybridization of biomolecules on the surface of the cantilever is investigated. The silicon-based cantilevers are typically of a micron order thickness doped with boron to introduce piezoresistivity. Microcantilever beams can be built as micro-mechanical arrays which could provide a basis for developing devices capable of performing multi-plexed, low-cost genomic and proteomic analyses. This paper provides several design solutions in optimizing the cantilever mechanical design to address the sensitivity required when approaching recognition of single base pairing of DNA molecules. The sensitivity of such piezoresistive cantilevers to the chemo-mechanical stress induced currents depends not only on the cantilever geometric properties, such as depth and width but also on the depth of the piezo layer (dopant) and its doping characteristics. It is often an expensive exercise to determine the optimum design parameters for increased sensitivity, particularly the dopant characteristics for such MEMS devices. A "managed solution" or parametric solution algorithm based on a finite element simulation is used to help determine optimum location and depth of this piezoresistive layer in the cantilever that maximizes the piezoresistor signals. Further, novel approaches for increasing the sensitivity of piezoresistive cantilevers through selected structural discontinuities are discussed.

Keywords: Piezoresistive cantilevers, stress concentration, MEMS, hybridization, unlabeled detection, parametric design, micro-mechanical array, Finite Element Analysis.

1. INTRODUCTION

Microcantilevers have been used to study surface stress as a result of adsorption of molecules. It has been demonstrated that microcantilevers are very sensitive to the adsorption of molecules and this has led to the use of microcantilevers as sensor devices for the detection of binding of mercury vapor, moisture, and volatile mercaptans [Thundat, T. et al., 1997]. More recently, microcantilevers have been used for the detection of adsorption and hybridization of biomolecules such as DNA [Thundat, T. et al., 1995], discrimination of single-nucleotide (SNP) mismatches in DNA [Fritz et al, 2000, Hansen, K.M., et al., 2001], protein binding [Moulin, A.M., 2000], and antibody-antigen binding [Thundat, T. et al., 2001].

A relatively simple and cheap mechanism for measuring binding-induced deflections in microcantilevers involves incorporating piezoresistive elements into the microcantilevers to measure cantilever stresses. Piezoresistive transducers are not new; they have been the method of choice for commercial accelerometers and strain gauges because they combine a linear response with a simple electrical output measurement. In experiments reported to date, deflections as small as 0.1 Å have been detected on individual microcantilevers using piezoresistive measurements [Tortonese et al., 1993].

The detection of biomolecules by a piezoresistive cantilever sensor depends on the relative change in resistance that is best measured by a Wheatstone bridge. For a given structure of a sensor (i.e., geometry and material), this change in resistance depends on differential stress between the top and bottom of the cantilever. This differential stress can result from binding of biomolecules, e.g., hybridization of DNA molecules to the side of the cantilever where adequate capture probes are attached. The mechanical differential stress will in turn result in change in the resistance of the piezoresistive cantilever and that resistance change can be measured in a very sensitive way by the Wheatstone bridge. Further, by measuring the resulting change in voltage across the bridge, it is possible to measure the amount of bio-molecules attached to the cantilever. Previous work suggests that a change in the magnitude of deflection of the cantilever is related to the DNA concentration on the surface [Fritz et al., 2000].

Although the detailed derivation is not given here, the fractional change in resistance ($\Delta R/R$) of a piezoresistive cantilever is described by the following expression:

$$\frac{\Delta R}{R} = \beta \frac{3\pi_L (1-\nu)}{t} (\sigma_1 - \sigma_2) \qquad \text{Equation (1)}$$

where π_L is the piezoresistive coefficient of Silicon along the <110> axis, σ_1 is the longitudinal stress, σ_2 is the transverse stress, t is the thickness of the cantilever, ν is the Poisson's ratio, and β is a factor that adjusts for the thickness of the piezoresistor [Harley and Kenny, 1999].

A close look at Equation (1) suggests that the relationship between the surface stress and the resistance change depends only on well-characterized physical constants and geometric factors. The ($\Delta R/R$) ratio can be increased by maximizing not the stresses, σ_1 and σ_2 separately as such but rather the difference (σ_1-σ_2). While the stresses themselves are directly related to the chemo-mechanical forces of biomolecule adsorption, it is, nonetheless, possible to increase the stress levels (selectively, if desired) by modifying the geometry of the micro cantilever. A number of novel methods such as reducing the depth at a location or introducing what are called SCR (stress concentration regions) across the plane of the cantilever are used to increase the stresses. The stress concentration region can be achieved by introducing openings (or holes) into the microcantilever structure. Such holes can be of different shape, e.g., elliptical, circular, square, and can be designed to occupy varying portions of the microcantilever detection surface. Thus, by introducing elliptical holes in the microcantilever as the SCRs, with their greater axis along the cantilever axis, and by biasing them in the longitudinal direction, one would obtain an increase in longitudinal stress, σ_1, and no noticeable change in transverse stress, σ_2. The overall difference, $\sigma_1 - \sigma_2$, increases, which in accordance with equation (1) will result in an increased resistivity detection signal.

Further, for a given geometry, the factor, β assumes a maximum value of 1.0 for extremely thin piezo layers and reduces to zero for piezoresistive layers extending through the entire depth of a cantilever. Therefore, it presents another design variable for increasing the sensitivity of the Wheatstone bridge. Other factors that affect the sensitivity include doping parameters (profile, depth, etc.), the fluid system, and the measurement electronics associated with noise reduction/identification method(s). All these variables present a mechanical and electrical design space that can be numerically simulated to arrive at parameters that will give optimum device operations and sensitivity.

2. DESIGN AND OPTIMIZATION OF PIEZORESISTIVE CANTILEVERS

As the piezoresistivity property of silicon is utilized to measure the mechanical stress induced in the cantilever due to adsorption or hybridization of analyte biomolecules, the sensitivity of the device can be enhanced significantly and its operations optimized by maximizing the piezoresistor signals.

In this study, we have developed a computational model (Finite Element Model) for simulating the electrical and mechanical response of piezoresistor cantilevers using CoventorWare™ from Coventor, Inc. The length of the cantilever shown in Figure 1 is 150 microns and it has a width of 40 microns and a depth of 1 micron. The finite element (FE) mesh consisted of a mesh of 4280 brick elements and 38415 nodes. Depth-wise, a fine mesh of 5 elements was used to accurately capture the stress gradient. The stress in the cantilever was modeled as a surface pre-stress of 0.5 MPa acting on a 200 Angstrom layer of Si Oxide on the top face of the cantilever.

Further, the following assumptions were made in the FE model:

1. The effect of temperature on conductivity of the piezo layer was ignored in the computational model even though the program used has a feature for accounting for the effect of change in temperature.

2. The effect of dopant-concentration on the electrical conductivity of the piezo layer was neglected. Again, if desired, the program used in this study provides a feature for modeling the dopant-concentration dependence.

Two of the key parameters that could be optimized in piezoresistor cantilevers (cf., Figure 1) are the geometry of the piezo layer and its doping characteristics. The length and location of the layer constitute the geometric components while the depth and profile of the doped layer constitute the doping characteristics. Regarding the length, location and depth of the piezoresistive layer, the following observations have a significant influence on the cantilever design decisions:

1. The stress induced in cantilevers due to binding or hybridization of biomolecules tends to be uniform throughout the capture area of the cantilever with noticeable peaks near the support [cf., Figures 2a and 2b]. This capture area (i.e., the surface of the cantilever where capture probes are placed) usually extends to the whole span of the cantilever. Therefore, the piezoresistive layer has to, preferably, extend over the capture area. This, however, is not an absolute requirement and, if desired, the piezoresistive layer could extend over at least one-third of the length of the cantilever to assure a big enough area for integrating the stresses.

2. Since binding and hybridization occur only on the face of the cantilever where capture probes are placed (usually only on one face), depth-wise, the stresses tend to vary in a triangular fashion from a maximum magnitude at this face to a minimum value in the opposite face. This suggests that the piezoresistive layer should never extend to the whole depth of the cantilever as the stress integral will reduce to zero. Further, this suggests that the piezoresistive layer should be as thin as possible and should be placed as close as possible to the face that contains the capture probes.

3. Results obtained from finite element analysis indicate a uniform stress distribution in the cantilever in both longitudinal and transverse direction under binding and hybridization induced chemo-mechanical forces. However, the distribution of the magnitude of the stresses in the longitudinal and transverse direction are different due to the geometry and boundary conditions [Figures 2 and 3]. This is confirmed by increasing the width of the cantilever to the same magnitude as the length effectively turning the cantilever beam to a cantilever plate. The differences in the longitudinal and transverse stresses reduced as geometry difference was removed. The fixed boundary condition which is symmetrical only in one plane, however, accounted for the still persistent difference between stresses in both directions. This is an important observation that has a bearing on the final design of the piezoresistors. A difference in longitudinal and transverse stresses suggests that p-type resistors (and not n-type) can be used effectively as shown below [10].

$$\Delta R/R = \Pi_{44} (\sigma_1-\sigma_2)/2 \qquad \text{Equation (2)}$$

where Π_{44} is the piezo coefficient and has a magnitude of 138.1 Mpa^{-1} for silicon.

The following design issues were addressed in the simulation.

1. The width of the piezoresistive layer is determined to be as close to the width of the cantilever as possible.

2. The length of the piezoresistive layer, on the other hand, does not necessarily have to be of the same length as the cantilever. For this particular study, we have limited the length of the piezoresistive layer to half of the cantilever length [i.e., 75 micron].

3. The location of the piezoresistive layer was varied by an increment of 15 microns and an automatic simulation run ("managed simulation") carried out to determine the location that corresponds to the maximum signal (i.e., current density, in our case). A plot of the variation of the current density in the piezoresistive domain with the shift in location of the piezoresistive layer is automatically generated by the program used (i.e., CoventorWare™ from Coventor, Inc). The geometry that corresponds to the maximum current density is then identified easily in a single run. The simulation runs confirm that the maximum possible signal is obtained when the piezoresistive layer is placed right at the clamped edge. This is expected as there is a noticeable stress concentration of about 10% increase at the clamped edges as shown in Figures 2.a and 2.b. Figure 6 shows the results of such a "managed solution" run. Figure 3 shows the variation of the longitudinal and transverse stresses along the width of the cantilever. Figures 4 and 5 show the current density distribution in the piezo layer with the maximum current density observed near the support and quickly vanishing towards the opposite end of the piezo layer.

4. The depth of the piezoresistive layer is limited to one-third of the depth of the cantilever due to practical consideration. A thinner doping depth would result in a β factor as close to 1.0 as possible.

Further, a "managed simulation" (or parametric simulation) is also carried out on the piezoresistive layer's electrical properties (i.e., conductivity) to determine an optimum electrical conductivity level for maximum signal. The conductivity was varied from -10% to 10% in steps of 10%. The sensitivity analysis indicates, as shown in the straight line in Figure 7, that the current density changes in the same ratio and direction as the change in electric conductivity.

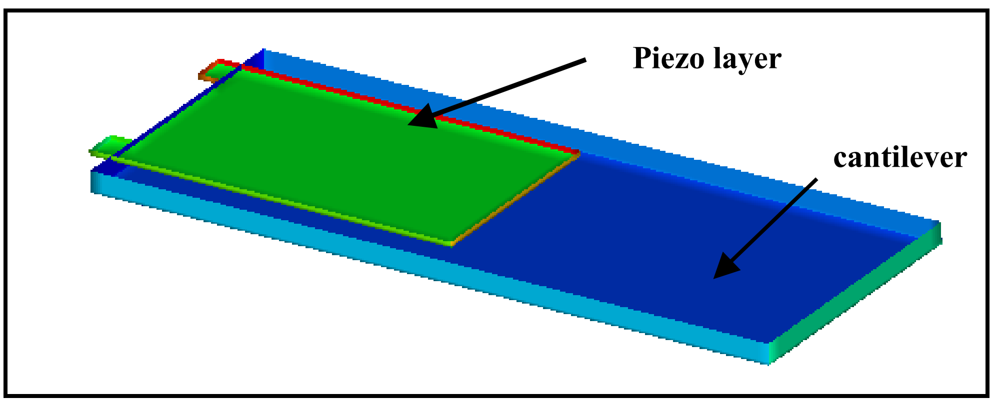
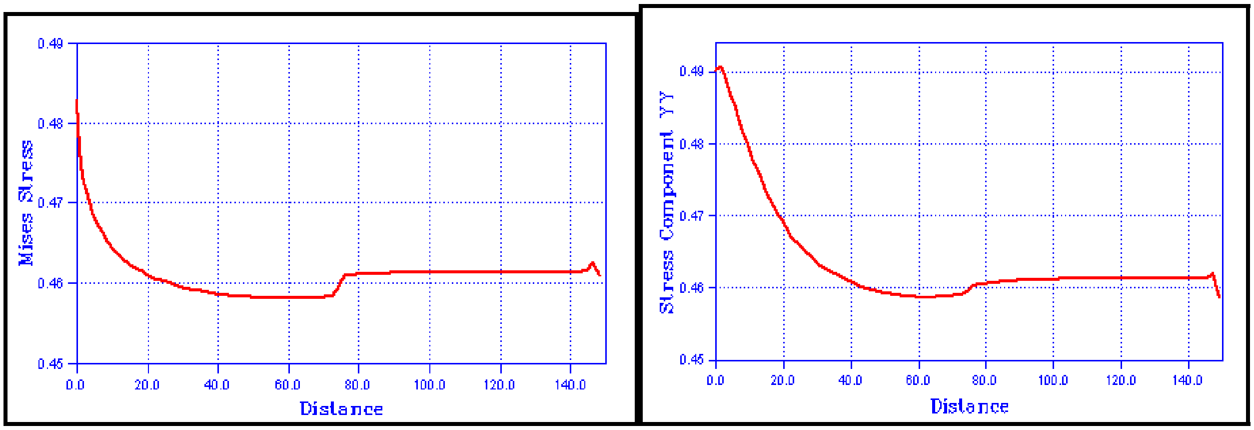


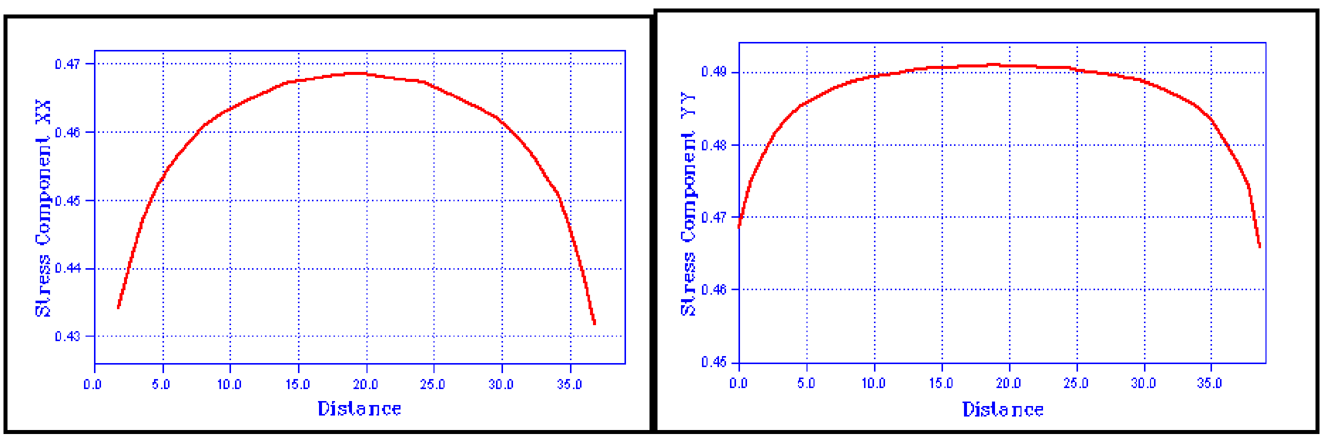
Figure 1. Cutaway view of a piezoresistive cantilever device.



a) Von Mises stress (MPa)

b) transverse stress - σ_2 (MPa)

Figure 2. Distribution of Von Mises and transverse stresses along the axis of a piezoresistive cantilever with distance in microns.



c) longitudinal stress - σ_1 (MPa)

b) transverse stress - σ_2 (MPa)

Figure 3. Distribution of longitudinal and transverse stresses along the width of the cantilever near the support.

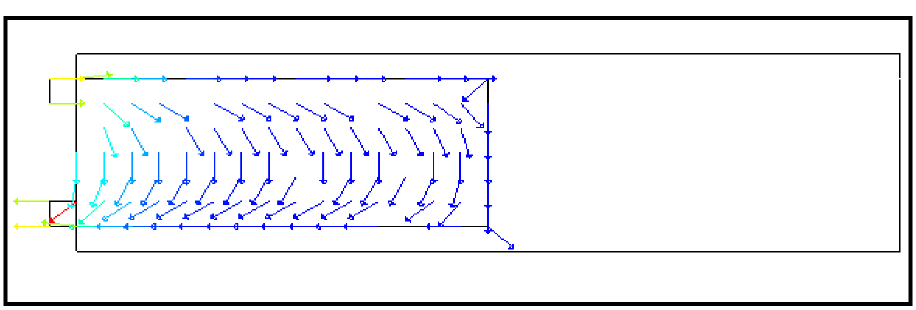


Figure 4. Current density distribution in a piezoresistive cantilever subjected to a surface stress.

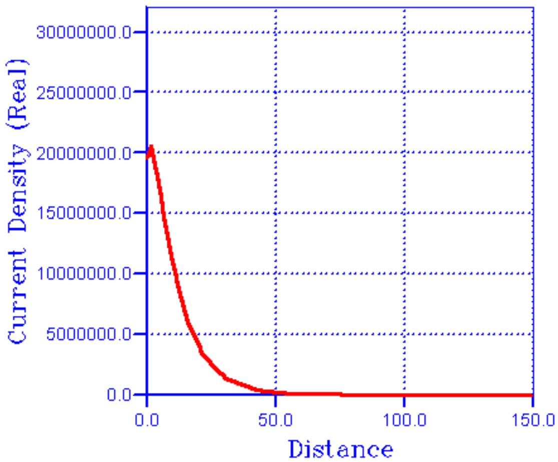


Figure 5. Longitudinal distribution of current density (pA/µm2) in a piezoresistive cantilever subjected to a surface stress.

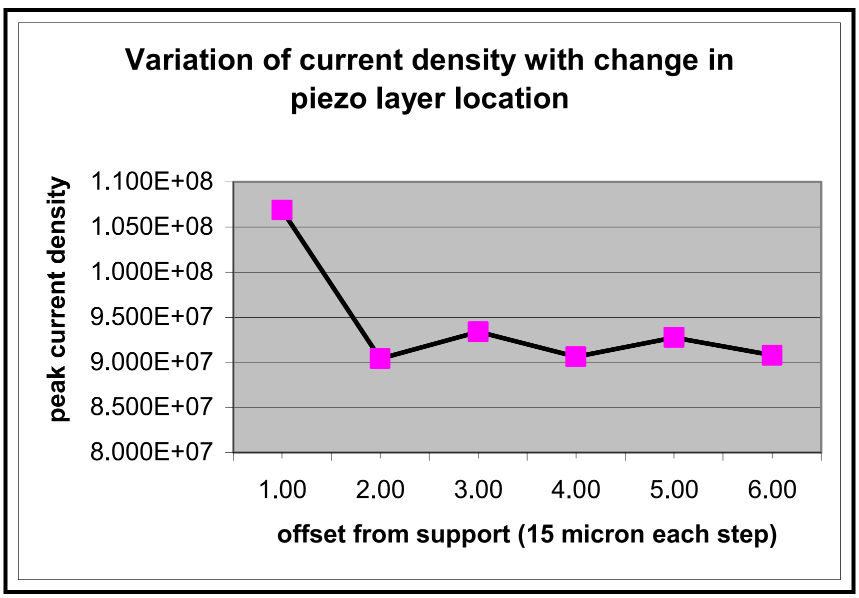


Figure 6. Variation of change in current density (pA/µm2) in a microcantilever with change in location of piezoresistive layer.

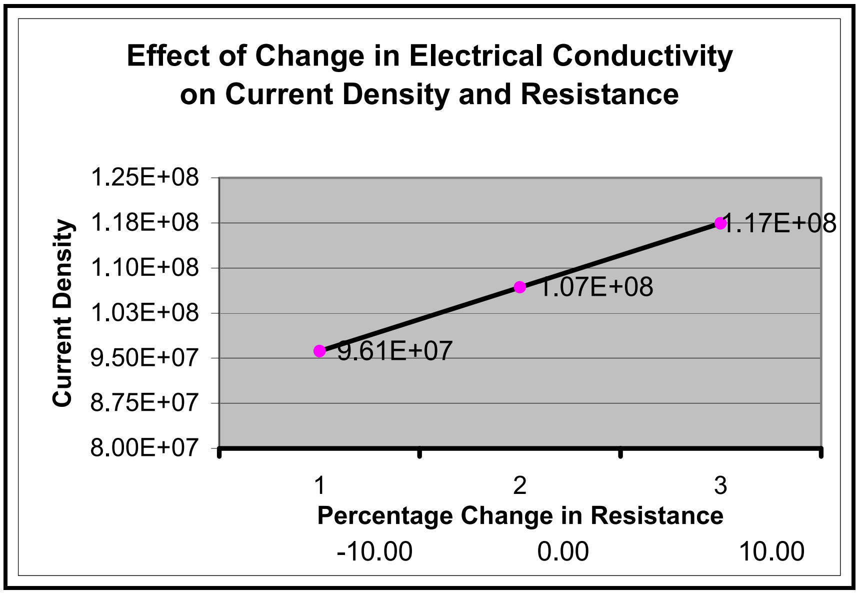


Figure 7. Variation of change in resistance in a microcantilever with change in electrical conductivity of piezoresistive layer.

3. INCREASING DEVICE SENSITIVITY THROUGH NOVEL METHODS

As shown in Equation (1), the mathematical relationship between the change in resistance dR in the piezo layer, and the longitudinal and transverse stresses, σ_1 and σ_2 suggest clearly that increasing the stress level itself will increase the dR/R signal in the piezoresistive layer.

In this work, we have investigated the implementation of the so-called "SCR" (stress concentration regions) such as structural discontinuities like holes and decrease in thickness near the base as possible means of increasing stress signals (hence change in resistance) in the piezoresistive cantilever device. Our simulation studies indicate that the introduction of thickness reduction in cantilever beams (near the base of the cantilever) can increases stresses in the range of 75-85% in both directions.

In addition, we have investigated stress increases due to structural holes placed in the cantilever. As pointed out earlier, the real value in increase in signal is realized by maximizing not the stresses, σ_1 and σ_2 separately as such but rather the difference (σ_1-σ_2).

Therefore, we have introduced rectangular and elliptical structural holes aligned in the longitudinal axis of the cantilever as shown in Figure 8. These discontinuities increase stresses disproportionally in the longitudinal and transverse directions resulting in a higher (σ_1-σ_2) difference that in turn increases the sensitivity of the piezoresistor. Figure 9 shows a magnified view of the increase in stresses at such discontinuities. Figure 10, on the other hand, shows the increase in current density signal in the piezoresistive cantilever. The presence of the holes increases the total area of the cantilever with significant current distribution, thereby resulting in higher signals. The increase in total integrated transverse stress in the piezoresistive cantilevers due to structural discontinuities is shown in Figure 11. This can be compared to Figure 2.b that represents the transverse stress for the whole cantilever with no structural holes; the significant increase being in the form of a widened area of stress peaks near the support which now extends to as much as 60 microns into the span of the piezo layer. Further note that, for example, that the stresses at the 20 microns, 40 microns and 60 microns locations of the cantilever with SCR have now increased to 0.48, 0.465 and 0.46 MPa as opposed to 0.4675, 0.46 and 0.456 MPa for the cantilever with no SCR.

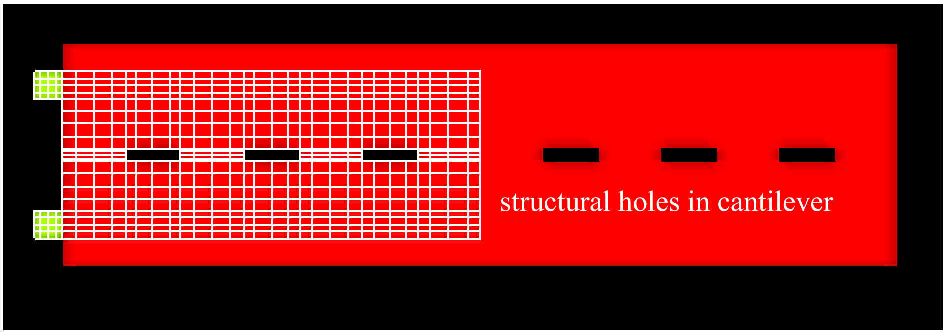
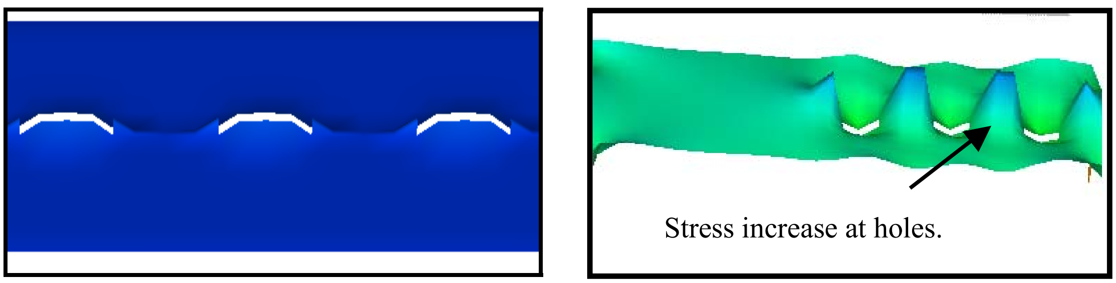


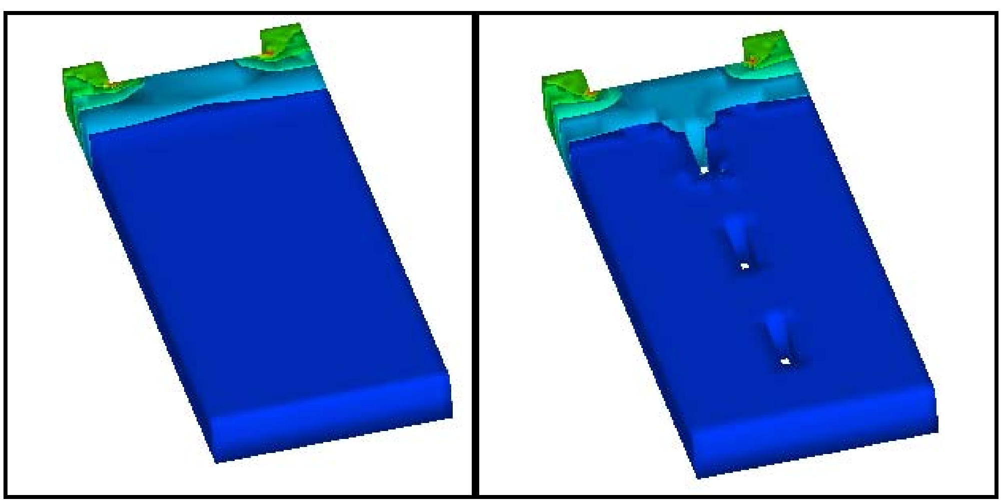
Figure 8. Stress Concentration in piezoresistive cantilever device can be achieved through structural discontinuities like holes.



a) Von Mises stress

b) transverse stress - σ_2

Figure 9. View of stress increases due to structural discontinuities.



a) contour of current distribution with no SCR

b) contour of current distribution with SCR

Figure 10. Increase in current density distribution in piezoresistive cantilevers due to structural discontinuities.

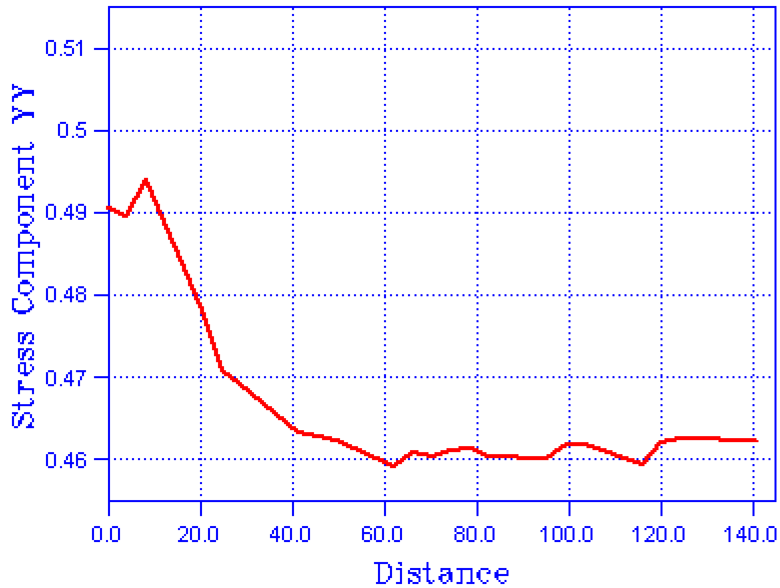


Figure 11. Increase in total integrated transverse stress (in MPa) in piezoresistive cantilevers due to structural discontinuities.

CONCLUSION

This work demonstrates that the optimization of the mechanical and electrical design parameters for micro piezoresistive cantilevers can increase the sensitivity of such devices enabling the detection of lesser amount of pathogens and biomolecules than currently possible. The use of a finite element method based simulation to arrive at optimally located piezoresistive layer is also demonstrated. The application of novel approaches for increasing the sensitivity of piezoresistive cantilevers through selected structural discontinuities is also demonstrated.

REFERENCES

1. Fritz, J., M. K. Baller, H. P. Lang, H. Rothuizen, P. Vettiger, E. Meyer, H.-J. Guntherodt, C. Gerber, J. K. Gimzewski. *Translating Bimolecular Recognition Into Nanomechanics.* Science, 2000. 288 (April): p. 316-318.
2. Hansen, K. M., H-F Ji, G. Wu, R. Datar, R. Cote, A. Majumdar, and T. Thundat. *Cantilever-Based Optical Deflection Assay for Discrimination of DNA Single-Nucleotide Mismatches.* Analytical Chemistry, 2001.
3. Harley, J. A. and T. W. Kenny. *High-Sensitivity Cantilevers Under 1000A Thick.* Applied Physica Letters, 1999. 75 (2): p. 289-291.
4. Moulin, A. M., S. J. O'Shea, M. E. Welland. *Microcantilever-Based Biosensors.* Ultramicroscopy, 2000. 82: p. 23 -31.
5. Thundat, T., P. I. Oden, and R. J. Warmack. *Microcantilever Sensors.* Microscale Thermophysical Engineering, 1997. 1089-3954/97: p. 1:185-199.
6. Thundat, T., L. A. Bottomly, S. Meller, W. H. Velander and R. Van Tassell. *Vapor Detection Using Resonating Microcantilevers.* Anal. Chem., 1995. 67(3): p. 519-521.
7. Thundat, T., L. A. Bottomly, S. Meller, W. H. Velander and R. Van Tassell. *Microcantilever Immunosensors*, in *Immunoassays: Methods and Protocols*, A.L. Ghindilis, A.R.Pavlov, and P.B. Atanajov, Editors. 2001, Humana Press: Totawa, N.J.

8. Stoney, G. Gerald. *The Tension of Metallic Films Deposited by Electrolysis.* Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character, Volume 82, Issue 553 (May 6, 1909), 172-175.
9. Tortonese, et. al. *Atomic Resolution with An Atomic Force Microscope Using Piezoresistive Detection.* Appl. Phys. Letters. 62(8), 22 February 1993.
10. Madou, Marc., Fundamentals of Micro-fabrication, CRC, 1997.