An optimised silicon piezoresistive microcantilever sensor for surface stress studies

Mohd. Zahid Ansari1 · Chongdu Cho2

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Abstract Surface stress is a versatile and efficient means to study various physical, chemical, biochemical and biological processes. This work focuses on developing high sensitive piezoresistive microcantilever designs to study surface stress. The cantilevers are made of silicon with rectangular holes at their base that also circumscribe a piezoresistor sensing element. To find the optimum design, the effects of change in cantilever width, rectangular hole length and type of dopant on mechanical properties like deflection, frequency and maximum stress are characterised using finite element analysis software. The surface stress sensitivity characteristics of the different cantilever designs is ascertained by applying a surface stress on their top surfaces. Results show that the sensitivity is increased by increasing the cantilever width as well as the length of the hole and the sensitivity of p-type designs is more than two times the n-type.

1 Introduction

Initially used in micro-electro-mechanical system (MEMS)-based pressure and acceleration sensors in 1960s, piezoresistive sensors have evolved considerably by the help of the developments in microfabrication techniques and nanotechnology to be of use in numerous modern sensor applications. The structure of piezoresistive sensors is generally cantilever or membrane type, with one or more doped piezoresistor elements inside. The sensors can be used to measure the mass change as well as the surface stress change. The present study will discuss the piezoresistive microcantilever sensors for surface stress studies. The measurement of surface stress variation using microcantilever sensor provides a very high sensitive, rapid and versatile means to study a variety of physical, chemical, biochemical and biological phenomena. The effects can be physical like moisture (Kapa et al. 2008), temperature (Lin et al. 2012) and thin film intrinsic stress (Wen et al. 2012); chemical like atrazine (Suri et al. 2008), explosive vapour sensor (Seena et al. 2011), trimethylamine sensor (Yang et al. 2010); bio-chemical like glucose (Chen et al. 2010), prostate specific antigen (PSA) protein (Lee et al. 2009), and Immunoglobulin G (IgG) (Yen et al. 2009) and biological like anthrax spores (Fu et al. 2007), severe acute respiratory syndrome associated coronavirus (SARS-CoV) (Velanki and Ji 2006), and bacterial virus T5 (Braun et al. 2004).

The sensitivity of a piezoresistive microcantilever sensor is defined in terms of its ability to convert the surface stress-induced external stimulus into resistance variation in its piezoresistor. The resistance can increase or decrease depending on the combination of the type of mechanical stress, i.e. tensile or compressive, and the transverse and longitudinal coefficients of piezoresistivity of the piezoresistor element. The sensitivity can be improved by cantilever design modification and changing the cantilever material. The cantilever design modifications include stepped and paddled designs (Ansari et al. 2012; Yang and Yin 2007; Mohammed et al. 2010; Zhang et al. 2011) and stress concentration regions (SCR) designs (Bashir et al. 2000; Wahid et al. 2013; Ansari et al. 2013; Ansari and Cho...
The cantilever material change can be changed to a softer one like SU-8 (Seena et al. 2011; Nordstrom et al. 2008) and SiO2 (Yang and Yin 2007; Zhou et al. 2009). In addition, sensitivity can also be improved by using the suitable type of dopant (Ansari and Cho 2014). In previous works, the authors has shown that the sensitivity of piezoresistive microcantilevers used in surface stress studies depends weakly on its length (Ansari and Gangadhara 2014) and inversely to its thickness (Ansari and Cho 2014). Hence, the present work focuses on determining the effect of increase in cantilever width on its surface stress sensitivity and on the combined effect of increase in width and the introduction of rectangular holes to induce high stress concentration regions in the designs.

The objective of the present study is to find the optimum cantilever design for improving the sensitivity of piezoresistive microcantilever for applications in surface stress studies. To simulate the surface stress, an in-plane bi-directional tensile force is applied to the top three free edges of the cantilever. The cantilevers are made of silicon with a doped piezoresistor inside. Four different cantilever designs in three modifications are investigated. The cantilever designs have different cantilevers widths and number of rectangular holes circumscribing the piezoresistor. The modifications are in form of the change in length of the rectangular holes. The piezoresistor width and thickness is kept constant. The piezoresistor type is changed as p-type and n-type. The sensing and reliability characteristics of the cantilever designs are studied and compared using a finite element analysis software.

2 Theory and modelling

Surface stress is a surface state wherein the outermost atomic layer of a solid is pulled inward by the underlying layers due to inter-atomic attractive forces. The absence of upper atomic layers results in a redistribution of electronic charges on the surface due to the change in the equilibrium positions of the atoms near the surface and a surface stress in the top layer is generated. Surface stress is an in-plane phenomena and is normally confined to few top atomic layers only. Surface stress is intrinsic to every surface and is generally of the order of 1 N/m on free metal surfaces. Surface stress-based sensors use the change in surface stress distribution on the surface due to the adsorption of foreign atoms onto its functionalized surface and the resulting stress and deflection to determine the quantities of interest.

In microcantilever sensors, the cantilever substrate is coated and functionalized with either a monolayer film of known receptor molecules or a thick solid film containing the receptor molecules. When the unknown analyte molecules are brought into contact with this active layer, analyte-receptor binding reactions takes place and the analyte is adsorbed onto the cantilever surface. This adsorption alters the surface stress distribution on the surface and produces stress and deflection in the cantilever which can be measured using optical deflection- and piezoresistive-readout techniques, respectively. The change is surface stress is generally less than 0.05 N/m.

In piezoresistive microcantilever sensors, the change in surface stress and the resulting deflection induces strain in the piezoresistor element of the cantilever and changes its electrical resistivity. Piezoresistivity is a material property which changes its bulk electrical resistivity when pressed. The piezoresistivity of a material is generally defined in terms of its average longitudinal ($\pi_x$) and transverse ($\pi_y$) linear coefficients of piezoresistivity. The coefficients depend on the type of dopant and its doping concentration. In addition, the coefficients also depend strongly on temperature. The total change in electrical resistance ($\Delta R/R$) of a piezoresistor with the current along the <110> axes, which is also the longitudinal direction of the piezoresistor and the cantilever, and subjected to longitudinal ($S_x$) and transverse ($S_y$) direction mechanical stresses in the piezoresistor can be given as

$$\Delta R/R = \pi_x S_x + \pi_y S_y.$$

Figure 1 presents the schematics of the proposed piezoresistive microcantilever designs as seen from above. The piezoresistor element layout is indicated in black. The basic model without the rectangular hole, i.e. Model#0, is also presented for a comparison. The geometric modifications in forms of introducing a rectangular hole, changing the piezoresistor length and changing the cantilever width are shown in the figure. Model#1 has three holes, Model#2 has five and Model#3 has seven identical holes. The width of piezoresistor leg is constant. The maximum tip deflection ($z_{\text{max}}$) in the cantilevers due to the applied surface stress ($\Delta \gamma$) on their top surface can be approximated as:

$$\Delta z_{\text{max}} = \frac{3K\Delta \gamma (1 - \nu) W}{E t^2} \left[ l - lL + (L - l)^2 \right]$$

where, $t$ is thickness, $W$ is total cantilever width, $W'$ is reduced cantilever width due to rectangular holes, $l$ is length of rectangular hole, $L$ is total length of the cantilever and $E$ and $\nu$ are the elastic modulus and Poisson’s ratio of the cantilever material. $K$ is a correction factor dependent on the material and geometric properties of the cantilever (Sader 2001).

3 Numerical analysis

The microcantilever designs proposed in this study were characterised numerically using commercial finite element analysis software ANSYS Multiphysics. The
designs were studied first for their structural integrity by determining the maximum cantilever tip deflection, fundamental resonant frequency and maximum von Mises stress, and then for their surface stress sensitivity by determining the average longitudinal and transverse stresses induced inside the piezoresistor element of the cantilevers. The geometric size of the proposed cantilever designs is shown in Fig. 1. Models#1–3 represent the increase in cantilever width and the introduction of rectangular holes in the cantilevers. The change in hole length is varied as 25 µm for A models, 50 µm for B models and 75 µm for C models. The width of hole is kept a constant at 20 µm. The piezoresistor is 10 µm wide and 0.1 µm thick, and is located at a depth of 0.1 µm from the top cantilever surface. The piezoresistors are changed as n-type and p-type.

Figure 2 shows the typical finite element model of the piezoresistive microcantilevers used in this study. The solid finite element models were meshed using 3-D coupled field 8-node scalar SOLID5 elements. Mesh convergence test was performed for a numbers of cases to confirm the validity of simulation results. On an average, more than 100,000 elements were used in each cantilever analysis. The cantilevers were subjected to three different loads simultaneously, i.e. a surface stress of 1 N/m which was applied to the top surface of the cantilevers, an ambient operating temperature of 25 °C with convective heat coefficient of air 200 W/m² °C and a bias voltage of magnitude 1 V. Surface stress was modelled as in-plane tensile force acting outward normal to the top three free edges of the cantilevers. The average longitudinal and transverse coefficients of piezoresistivity ($\times 10^{-11}$ m²/N) are, respectively, $-31$ and $-18$ for n-type, and $+72$ and $-66$ for p-type (Tuft and Stelzer 1963). The mechanical properties are listed below in Table 1.
4 Results and discussion

Figure 3 presents the numerical results for maximum cantilever tip deflection, fundamental resonance frequency and the maximum von Mises stress induced in the cantilever designs when subjected to 1 N/m of surface stress on their top surfaces. The deflections increase with increase in length of the rectangular holes as well as the cantilever width. The increase can be attributed to the decrease in their bending stiffness due to the presence of holes at the fixed end. The increase in hole length is, however, much more effective in increasing the deflection. The frequency results, however, show a pattern opposite to the deflection case. The frequencies decrease with increase in hole length as well as cantilever width. Interestingly, the frequency results for the base models, i.e. A0, B0 and C0, are almost same. This suggests the increase in cantilever width has negligible effect on the frequency. This observation can also be observed in the other cantilever models to a lesser extent. This behaviour can be explained by the fact the increase in cantilever width is increasing linearly both the bending stiffness as well as the cantilever mass. However, since the frequency is directly proportional to the in square root ratio of cantilever stiffness and its mass, the width term in the two quantities cancels out. Therefore, the increase in cantilever width has negligible effect on its frequency. The high frequency of the base models can be attributed to their high bending stiffness because of no holes at the fixed end.

The results for maximum stresses induced in the cantilevers are also presented in Fig. 3. The introduction of holes is clearly amplifying the amount of stress induced in the cantilevers. However, since the maximum stresses inside the cantilevers are well below their fracture strength of about 300 MPa (Sooriakumar et al. 1995), the designs...
presented in this study are safe from fracture failure. In addition, since the typical values of surface stress encountered in analyte-receptor bonding reactions are less than 0.05 N/m, which is one-twentieth the value used here, the deflection and stress induced in the cantilevers would diminish accordingly.

Figure 4 presents the comparison between the average stress values induced in the piezoresistor element along its longitudinal and transverse directions for the different cantilever designs when subjected to 1 N/m surface stress. The difference in the two stress values is also plotted. It is obvious in the figure that the introduction of the rectangular hole at the fixed end in the base models alone increases the longitudinal stress in models A1, B1 and C1 by about 1.74, 1.80 and 2.65 times their respective base model results. The transverse stress values in these cases, however, show a decrease in A1 and B1 but a slight increase in C1. The increase in hole length is clearly increasing the stress values in both direction. The rate of increase in longitudinal stress is, however, much higher than the transverse stress.

The increase in cantilever width is increasing the longitudinal stresses but decreasing the transverse stresses induced in the piezoresistor. The increase can be attributed to the higher deflections produced in these cantilevers. And, the decrease can be attributed to the relative less rigorous displacement constraint boundary length imposed to the cantilever width at the fixed end. Since the sensitivity of a piezoresistive microcantilever biosensor depends on the resistance change induced in the piezoresistor whose magnitude depends on the longitudinal and transverse stresses, the stress difference values are also plotted in Fig. 4 to show the effects of the presence of rectangular hole and the hole length as well as the cantilever width. It can be seen in the figure that the stress difference values are increasing with all the three modifications.

Figure 5 shows the normalised surface stress sensitivity results for the n-type and p-type piezoresistive microcantilever biosensors under a surface stress of 1 N/m. The standard sensitivity of A0 model for n-type and p-type microcantilevers, which is used to normalise the other results, is about $-0.132$ and $+0.102$ %, respectively. The negative sign for n-type indicates that the total electrical resistance is decreasing which is because of its negative coefficients of piezoresistivity. Though the n-type basic microcantilever design A0 has a higher absolute sensitivity than corresponding p-type, the geometric modifications incorporated

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**Fig. 4** Comparison between average values of longitudinal stress, transverse stress and its difference in the piezoresistor of different cantilever designs.

**Fig. 5** Comparison between normalised sensitivity results in n-type (left) and p-type (right) cantilever designs.
to improve further the sensitivity are less helpful in case of n-type, as shown in Fig. 5.

The increase in cantilever width of n-type cantilevers is decreasing its sensitivity, whereas, it is increasing first and then decreasing in case of p-type. This is because of the combined effect of increase in longitudinal and decrease in transverse stresses in these cantilevers (see Fig. 4). In addition, since the longitudinal and transverse piezoresistive coefficients of n-type and p-type piezoresistor have different magnitudes and symbols, the contributions to the total resistance change, i.e. sensitivity, are additive for n-type but subtractive for p-type cantilevers. The introduction of rectangular holes increased the sensitivity of A1, B1 and C1 designs to about 1.5, 1.9 and 2.3 times for n-type and 2.9, 2.7 and 3.7 times for p-type cantilevers than their base models A0, B0 and C0. The effect of increase in hole length in these designs, however, has less significant effect and the maximum improvement is less than 23 % for n-type and 28 % for p-type cantilevers.

The maximum increase in sensitivity achieved in n-type design by means of introducing the geometric modifications is about 80 %. In contrast, the same results for p-type show a maximum increase of about 340 %. Based on the results shown in Fig. 5, we can conclude that the sensitivity of piezoresistive microcantilevers can be significantly increased by incorporating the geometric modifications in form of high width and rectangular holes. Though Model#3 cantilevers are showing the highest sensitivity, the fabrication of such designs may be a challenging task. In general, fabrication of narrow cantilevers is easier than a wide one from the release point of view. In addition, cantilevers with long rectangular holes can have a higher probability of non-zero initial deflections and stresses. Therefore, considering the microfabrication constraints we can conclude that p-type B2 microcantilever is the most suitable design for improving the sensitivity of the piezoresistive microcantilever for surface stress studies. This design is relatively easy to fabricate and is less susceptible to fabrication-induced residual stresses.

5 Conclusions

This study investigated new silicon piezoresistive microcantilever designs for surface stress studies application using finite element analysis software. The objective was to find the optimum design of the cantilever for such a study by varying the cantilever width, introducing rectangular hole and increasing the hole length, and by changing the type of piezoresistor. The designs were characterised for their tip deflection, resonant frequency, maximum stress and surface stress sensitivity. The surface stress sensitivity of each design was determined by determining the average longitudinal and transverse stress in their piezoresistor element. Results showed that the increase in the cantilever width has mixed results on sensitivity. The sensitivity decreased with increase in cantilever width for n-type designs, and first increased then decreased for p-type designs. The introduction of rectangular holes in the base designs A0, B0 and C0 increased their sensitivity by about 50 % in n-type and 190 % for p-type designs. However, when the increase in width is combined with the increase in rectangular hole length, the sensitivity of the base designs A0, B0 and C0 is improved by about 70, 90 and 130 % in n-type, and 190, 170 and 270 % in p-type, respectively. In addition, the increase in hole length was found to have less significant effect on increasing sensitivity and the maximum improvement is less than 23 % for n-type and 28 % for p-type cantilevers. We found that the maximum increase in sensitivity achieved by means of introducing the geometric modifications is about 80 % in n-type and 340 % for p-type designs. Considering the design requirements of high resonant frequency, high sensitivity and fabrication challenges, we can conclude that p-type B2 microcantilever is the most suitable designs for surface stress studies.

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