Simulation of SiO₂-based piezoresistive microcantilevers

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Abstract

This article uses finite element design for optimization of piezoresistive Si covered SiO₂ microcantilevers. The maximum resistance changes were systematically investigated by varying piezoresistor geometries and doping concentration. Our simulation results show that both cantilever deflection displacement and \( \Delta R/R \) change decrease when the thickness of piezoresistors increases; the highest sensitivity can be obtained when the piezoresistor length is approximately 2/5 of the SiO₂ cantilever length; increase of both Si width and leg width result in decrease in cantilever deflection and sensitivity; the sensitivity of cantilevers with lower doping concentrations is more significant than those with higher doping concentrations. Temperature control is critical for thin piezoresistor in lowering the S/N ratio and increasing the sensitivity.

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1. Introduction

Microcantilevers have proven to be an outstanding sensor platform for extremely sensitive chemical and biological sensors [1–20]. Piezoresistance-based microcantilever transducers are becoming increasing popular in recent years as they are convenient to calibrate, readily deployable into integrated electromechanical system and do not require external detection devices for measuring surface stress as a result of the binding of chemical and biological species [21–23]. All these advantages come at the expense of lower resolution than the optical-based system. Previously, attempts were made to improve the sensitivity and resolution of piezoresistive microcantilevers by reducing the thickness of the cantilevers [24] and by incorporating stress concentration regions [25], etc. Investigations of piezoresistor sensitivity to noise were also reported [26–29]. These articles provided strong foundation for silicon-based piezoresistive cantilever transducers.

Recently, we reported that SiO₂ microcantilevers offer approximately 20-fold deflection amplitude compared to that of silicon microcantilevers with the same dimensions when the same surface stress is applied [30]. Furthermore, such SiO₂ microcantilevers were extremely useful in detection of HF and nerve agents [31]. Our previous work focused on laser optical approach for cantilever deflection measurements. In order to eliminate the complexity inherent to optical instruments, which require laser system adjustment, we are to develop piezoresistive cantilevers for future hand-held sensor device. No simulation work has been done on SiO₂-based piezoresistive microcantilevers. This article uses popular finite element analysis approach to simulate the geometrical parameters and process conditions for SiO₂-based piezoresistive microcantilevers. A thin layer of boron-doped Si on the SiO₂ surface was used as piezoresistive materials. Finite element model was developed to analyze electrical and mechanical response of piezoresistor cantilevers by using CoventorWare (Coventer Inc., Cary, NC). Calculation results on the displacements and the \( \Delta R/R \) changes of the cantilevers were also discussed as a comparison to the simulation results.

2. Analytical model

The geometry of a SiO₂-based piezoresistive microcantilever is shown in Fig. 1.

The surface stress on the microcantilever surface can be calculated from the observed cantilever deflection using Stoney’s equation [12]:

\[
\Delta \sigma = \frac{E h^2}{6(1-\nu) r}
\]  

(1)
where $\Delta \sigma_s$ is the differential surface stresses on the surface of the microcantilever, $E$ the Young’s modulus, $\nu$ the Poisson’s ratio, $r$ and $h$ are the radius of curvature and thickness of cantilever beam, respectively.

For a two-layer piezoresistive microcantilever, the relationship between the surface stress and the relative change in resistance $\Delta R/R$ for a piezoresistor is given by \[32\]

$$
\frac{\Delta R}{R} = -K \left( \frac{1}{E_1 h_1 + E_2 h_2} \right) \times \Delta \sigma_s,
$$

(2)

where $E_1, h_1$ are the Young’s modulus and thickness of the SiO$_2$, respectively, $E_2, h_2$ the Young’s modulus and thickness of the Si piezoresistor, respectively, $Z_T$ the distance from neutral axis to top of the cantilever beam containing piezoresistor, and $K$ the gauge factor of piezoresistor (=140). However, the above equation only applies when the length of the Si piezoresistor is same as the SiO$_2$ cantilever length.

3. FEM analysis and optimization

The MemPZR module in CoventorWare computes the change in resistivity of a piezoresistive material subject to mechanical deformations through finite element method (FEM). The piezoresistive phenomenon in semiconductors is linked to a change in resistivity of the silicon materials in response to an applied stress. Ohm’s Law in the stress-free state represents this effect mathematically [33]:

$$
\begin{bmatrix}
E_1 \\
E_2 \\
E_3
\end{bmatrix}
= \rho_0
\begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{bmatrix}
\begin{bmatrix}
i_1 \\
i_2 \\
i_3
\end{bmatrix},
$$

(3)

where $E_i, i$ are the electric field and current density, respectively, parallel to the $x_i$ crystallographic axis and $\rho_0$ is the stress-free resistivity, which may be tensor in general.

When a stress field is applied, the resistivity is modified and becomes anisotropic. Sader [33] reported previously that, application of differential surface stress to a rectangular plate is equivalent to loading of the free edges by moments per unit length of magnitude $\Delta \sigma_s h/2$. When applying for boundary conditions to the meshed model, the above result was used.

The application of surface stress causes the microcantilever resistivity to change. The change in resistivity is related to the surface stress through the empirically determined piezoresistive coefficient. For the silicon material, there are three independent piezoresistive coefficients $\pi_{11}, \pi_{12}$, and $\pi_{44}$, where the subscripts physically represent the electric field, current density, and stress along the three crystallographic directions for cubic crystal silicon. The change in resistivity is related to the surface stress through the empirically determined piezoresistive coefficient. The material properties are listed in Table 1 [34].

4. Results and discussion

4.1. Effect of thickness of piezoresistor on cantilever displacement and sensitivity ($S = \Delta R/R$)

The cantilever sensitivity ($S$) can be expressed as fractional change in resistance of the cantilever ($\Delta R/R$). Cantilever thickness.

### Table 1

<table>
<thead>
<tr>
<th>Material property</th>
<th>Material property of silicon with surface stress at [1 1 0] direction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus (MPa)</td>
<td>$1.30 \times 10^5$</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>0.278</td>
</tr>
<tr>
<td>Shear modulus (MPa)</td>
<td>$7.96 \times 10^4$</td>
</tr>
<tr>
<td>Density (kg/m$^3$)</td>
<td>$2.33 \times 10^3$</td>
</tr>
<tr>
<td>Thermal coefficient (pW/°K)</td>
<td>$1.48 \times 10^8$</td>
</tr>
<tr>
<td>Resistivity ($\Omega$ cm)</td>
<td>7.8</td>
</tr>
<tr>
<td>Young’s modulus (MPa)</td>
<td>$7.0 \times 10^3$</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>0.17</td>
</tr>
</tbody>
</table>
ness is a crucial parameter that affects the detection sensitivity. The dimensions of the designed SiO$_2$ cantilevers are 250 $\mu$m in length, 100 $\mu$m in width, and 1 $\mu$m in thickness. Finite element analysis shows that both cantilever deflection displacement and sensitivity increase when the thickness of piezoresistors decreases from 2 to 0.2 $\mu$m (Fig. 2). The figures were obtained by applying a 2 N/m surface stress on the surface of the cantilever and piezoresistor. A 2 N/m surface stress was used in this study because the surface stress changes at this level have been typically observed in many microcantilever chem/biosensors.

The $\Delta R/R$ keeps increasing when the thickness decreases. This is probably due to (a) larger bending when the Si resistor is thinner (its Young’s modulus is 180 GPa compared to that of 70 GPa of SiO$_2$ cantilever) and/or (b) the resistivity change is larger for thin Si materials because of quantum size aspects of the piezoresistor [35]. The optimized thickness for chem/bio sensing, however, could be obtained from a noise optimization.

Piezoresistive sensors have two main possible noise sources, thermal and Hooge noise, which are generated from temperature and voltage variations, respectively [36]. Larger noise will lower the signal/noise (S/N) ratio, and thus the sensitivity. Understanding the effects of temperature and voltage variations on the S/N ratio will help us to optimize the thickness of piezoresistive cantilevers. Fig. 3a shows that a 0.3% voltage variation does not change the $\Delta R/R$ of the cantilever. However, a 0.3% temperature variation (Fig. 3b) causes significant noises, especially when the Si piezoresistor is thinner than 1 $\mu$m, suggesting that thermal variation is the major source of the sensor noise.

Fig. 3b inside shows the resistance change noise because of the 0.3% temperature variation (defined as $\Delta R/R_{299K} - \Delta R/R_{298K}$). The noise of the resistors jumps approximately 10-fold when the thickness is from 1 $\mu$m to 0.2 $\mu$m. From those data in Figs. 2b and 3b inside, the S/N ratio of the microcantilever at different thicknesses can be calculated as shown in Fig. 4. These results suggest that although the $\Delta R/R$...
of the cantilever increases when the thickness decreases, the optimized S/N ratio can be obtained when the thickness Si piezoresistor is 1.2 μm when 1 K temperature variation (from 298 to 299 K) is considered. Temperature control is critical in lowering the S/N ratio and increasing the sensitivity. It is anticipated that when the temperature variation is small, thin Si piezoresistor can be used for sensing application that will give better ΔR/R without sacrificing the S/N ratio.

4.2. Effect of Si piezoresistor length on the cantilever displacement and sensitivity

When a surface stress is applied on a cantilever, the deflection amplitude increases from the support end to the free end of the cantilever. So, the longer the piezoresistor (Lp), the larger the ΔR/R is expected; on the other hand, when Lp increases, the cantilever deflection amplitude will decrease due to the large spring constant of the piezoresistor (Fig. 5a). Thus, it is a necessity to investigate the effect of Lp in order to obtain the maximum ΔR/R.

Fig. 5b shows that the maximum ΔR/R was obtained when the piezoresistor length is approximately 2/5 of the SiO2 cantilever length. The ΔR/R decreases when the length is extended beyond 100 μm. It was also observed that ΔR/R changes have similar trends for different thicknesses of the piezoresistor, and ΔR/R changes are more significant for cantilevers with thinner Si piezoresistors.

To further support the conclusions, the effects of piezoresistor length on ΔR/R of a longer SiO2 cantilever with 500 μm in length were investigated. Finite element analysis shows (Fig. 6) that maximum ΔR/R can be obtained when the Lp is approximately 2/5 of the SiO2 cantilever length.

4.3. Effect of piezoresistor width on microcantilever displacement and ΔR/R

It has been reported previously from both experiments and finite element analysis that the microcantilever deflection could be affected by the cantilever width [36,37]. However, the effect
of piezoresistor width on cantilever deflection and $\Delta R/R$ has not been investigated.

Our finite element analysis shows that the width of the piezoresistor also plays a role in the piezoresistive cantilever sensitivity. The increase from 10 to 30 $\mu$m width resulted in 15% and 74% decrease in cantilever deflection and $\Delta R/R$, respectively (Fig. 7). The decrease in the cantilever deflection and $\Delta R/R$ can be explained by the spring constant increase due to the increase of resistor width.

From the above calculation and hypothesis, we anticipate that the distance between the two piezoresistor legs will also affect the cantilever sensitivity. Finite element analysis proved that an increase in leg width slightly decreases the fractional change in resistance as shown in Fig. 8. The analysis was carried out by keeping the piezoresistor width constant at 20 $\mu$m.

### 4.4 Fabrication process

The designed fabrication process has four steps: first, pattern the piezoresistor on top Si of the SOI wafer by photolithography and dry plasma etching; second, pattern the cantilever beam on the buried SiO$_2$ layer by the second photolithography process and buffered oxide etching (BOE); third, pattern the electrode on the SiO$_2$ surface by the metallization and “lift-off” method; fourth, release the cantilever from bulk silicon by dry plasma etching.

The fabrication process of SiO$_2$ supported piezoresistive cantilevers is shown in Fig. 9. Shipley 1813 positive tone photoresist was spun on the surface of SOI wafer (Fig. 9a). A piezoresistor pattern was transferred to the photoresist layer on the top side of the wafer by standard photolithography process and then the Si piezoresistor was formed by inductive coupled plasma (ICP) etching (Fig. 9b). The photoresist was then cleaned by acetone and DI wafer. A layer of 1813 photore sist was spun on the surface of the buried oxide layer of the SOI wafer. The microcantilever beam pattern was transferred to the photoresist layer and then the SiO$_2$ cantilever beam were formed by etching with buffered oxidation etchant (BOE HF:HNO$_3$ $=$ 1:6). The photoresist was then cleaned by acetone and DI water (Fig. 9c).

Next, a modified photoresist LOR lift-off processing was employed for contact electrode pad fabrication. Firstly, a layer of LOR 7B was spin-coated on the wafer, followed by a layer of 1813. The electrode pattern was transferred to the photoresist layer. Because LOR B series have relatively high dissolution rates, undercutting appears and the lift-off undergoes readily. A thin film of gold is deposited by the sputtering. Ultrasonic was used to remove the photoresist, leaving the gold pad on the SiO$_2$ (Fig. 9d). Finally, a 20-μm-thick photoresist AZ9260 was spun on the backside of the wafer and followed with typical photolithography pattern process. The thick photoresist pattern served as a mask for deep silicon plasma etching. The Si was etched off by inductive coupling plasma (ICP) process to release microcantilever beams from bulk silicon (Fig. 9e).

The silicon resistor and SiO$_2$ layer of the commercially available ROI wafer in our experiment were 2 and 1 $\mu$m in thickness, respectively. The SEM picture of a fabricated cantilever is shown in Fig. 10. Our preliminary data showed that the resistance of the piezoresistive cantilever changed from 1.5734 to 1.5738 M$\Omega$ upon exposure to a 100% saturated water vapor, i.e. 0.03% change of the resistance ($\Delta R/R$). The saturated water vapor could generate a close to a 2 N/m surface stress on the cantilever surface. This result matched very well with our simulated results. The detailed characterization of the cantilevers with different Si thickness are under investigation and will be reported in due time.
5. Conclusion

Finite elements analysis was used to optimize the performance of Si covered SiO₂ cantilevers. Various parameters, such as thickness, length, width, doping concentration, that affect the resistance changes of the piezoresistive cantilevers were thoroughly investigated. The results could provide guidance to fabrication of optimized SiO₂-based piezoresistive cantilevers. The best sensor performance is expected to be achieved when the Si piezoresistor is thin, narrow, low doping level, and when the piezoresistor length is approximately 2/5 of the SiO₂ cantilever length. Temperature control is critical in lowering the S/N ratio and increasing the sensitivity. It is anticipated that when the temperature variation is small, thin Si piezoresistor can be used for sensing application that will give better $ΔR/R$ without sacrificing the S/N ratio.

Acknowledgments

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