

Modelling the Piezoresistive Mems Cantilever for Chemical Sensing

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Abstract: MEMS (Micro Electro Mechanical Systems) sensors are used in acceleration, flow, pressure and force sensing applications on the micro and macro levels. Much research has focused on improving sensor precision, range, reliability, and ease of manufacture and operation. Over the last 15 years, researchers have explored the use of piezoresistive microcantilevers/resonators as mass sensors because of their relative ease in fabrication, low production cost, and their ability to detect changes in mass or surface stress with fairly good sensitivity. However, existing microcantilever designs rely on irreversible chemical reactions for detection and researchers have been unable to optimize symmetric geometries for increased sensitivity. The cross-sensitivity of microcantilever sensors presents a major obstacle in the development of a commercially viable microcantilever biosensor for point of care testing. The presented paper aims to optimize the performance of piezoresistive cantilevers in cases where the output signal originates either from a static deflection of the cantilever. The presented optimizations for the static mode specifically targets the force sensitivity of piezoresistive cantilevers.

Keywords: MEMS, Cantilever, Piezoresistive, Deflection

I. INTRODUCTION

A fundamental part of every sensor is the transducer, which converts the measure and of interest into an interpretable output signal. One of the most prominent transducers in the micro-realm is the piezoresistive cantilever, Which translates information from the mechanical into the electrical domain, e.g. the amount of force exerted on the cantilever into a resistance

change or the amount of mass added to the cantilever. As the title of this thesis suggests, this research focuses on the application of piezoresistive cantilevers in static mass sensing. In other words, the presented work aims to optimize the performance of piezoresistive cantilevers in cases where the output signal is DC (e.g., strain gauges) signal. While the presented research for the static mode specifically targets piezoresistive cantilevers, the optimization results and findings for the dynamic mode can be extended to cantilevers with other sensing schemes. In general, most of the MEMS biomass sensors are used for sensing picograms to femtograms of weight (e.g. mass of E.Coli. bacteria). But, these molecules (i.e., acetone, ethanol, etc.) have to be sensed using a cantilever with more sensitivity and stiffness. Thus, this work focuses on building a MEMS cantilever with improved sensitivity and stiffness of the cantilever.

II. DESIGN OF PIEZORESISTIVE FORCE SENSING CANTILEVER

In this part, for measuring point loads at the free end, design criteria for cantilever sensors optimized are discoursed. Applications of this kind of measurement technique could embrace Nano indentation and bio molecular force measurements from simple two-dimensional considerations, the stress in the cantilever x-direction can be derived as a function of the position in the beam.

$$k = \frac{F}{\delta} = \frac{W_c \cdot t_c^3 \cdot E_c}{4l_c^3}$$

Where F is the applied point force at the free end, and w_c , t_c and l_c are cantilever width, thickness, and length, respectively. The two-dimensional model assumes that stress in the y-direction σ_y is always linearly related to σ_x through $\sigma_y = -\nu \cdot \sigma_x$. Thus, for a piezo-resistor along the cantilever length direction ($\sigma_l = \sigma_x$; $\sigma_t = \sigma_y$), the stress difference $\Delta\sigma_l$ is

$$\Delta R/R = \pi_{lt} \frac{12}{w_c t_c^3} \left(l_c - \frac{1}{2} l_p \right) \left(\frac{t_c}{2} - \frac{t_p}{2} \right) F$$

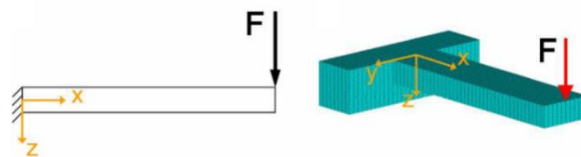


Fig. 1(a) Design for measuring point load at free end of the cantilever

The cantilever length, width and thickness are chosen to be 200 μ m, 100 μ m, and 2 μ m, respectively. The external areas of the anchoring substrate, except for side that the cantilever is attached to and the top side, are fully constrained. Figure shows the comparison of FEM simulations of stress distributions in x- and y-direction from the analytical solution and the x-z-plane

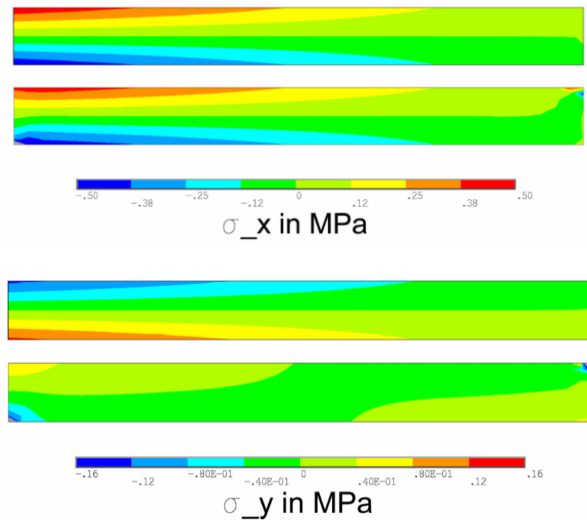


Fig. 1(b) Figure shows the comparison of FEM simulations of stress distributions in x- and y-direction from the analytical solution and the x-z-plane

By the analytical model the stress in x-direction is anticipated in both its magnitude and distribution well. The only differences in the FE model are the stress concentrations due to the point force at the cantilever free end and smaller degree at the clamping, which are not deliberated in the analytical solution. The stress in y-direction differs ominously between the two models due to the more pronounced effect the clamping has on the stress in this direction. Only two solutions show good agreement far away from the clamping and not directly at the free end. The analytical solution still has some validity because the stress in x-direction is much higher than the stress in y- direction however, if the stress difference is the significant parameter and it agrees with the FE model. The resistance change $\Delta R/R$ of a piezo-resistor within the cantilever can be determined from the stress distribution. Supposing that the current direction within the cantilever is in the direction of the cantilever length. The average resistance change can be calculated by integrating equation over the piezoresistive area for the analytical model, dividing by that area, and plugging the result into equation which can be given as

$$\frac{\Delta R}{R} = \pi_{lt} \frac{1}{(x_2 - x_1)(z_2 - z_1)} \int_{x_1}^{x_2} \int_{z_1}^{z_2} \frac{F \cdot 12 \cdot (1 + \nu_c)}{w_c t_c^3} (l_c - x) z dz dx$$

Where (x_1, z_1) and (x_2, z_2) are two opposite corners of a rectangular piezoresistive element within the cantilever. For the FE model, equations or can be used within each element in the piezoresistive area and the results are averaged above all elements. A more realistic cantilever geometry than in Figure 1(a), i.e. a device with smaller thickness, was chosen to parallel the results from the analytical model to the FE model for the resistance change.

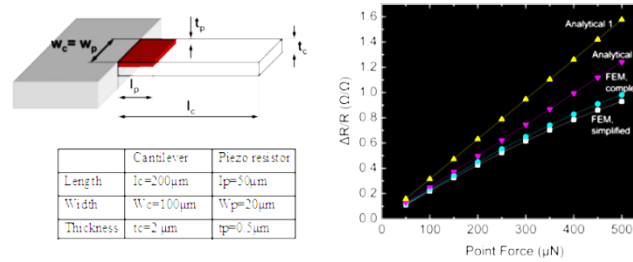


Fig.2Cantilever Geometry

From the geometries of cantilever and piezoresistor as shown in Figure equation becomes

$$\begin{aligned} \delta &\underset{(1,5)}{=} \frac{l_c^2}{2r} \underset{(1,2)}{=} \frac{l_c^2}{2} \frac{6(\Delta\sigma_1 - \Delta\sigma_2)}{M_c t_c^2} \underset{(1,3)}{=} \frac{l_c^2}{2} \frac{6(1-\nu)(\Delta\sigma_1 - \Delta\sigma_2)}{E_c t_c^2} \\ &\underset{(1,17)}{=} \frac{\Delta R}{R} = \beta \pi l_t \frac{3E_c t_c}{2l_c^3} \left(l_c - \frac{1}{2} l_p \right) \frac{l_c^2}{2} \frac{6(1-\nu)(\Delta\sigma_1 - \Delta\sigma_2)}{E_c t_c^2} \\ &= \beta \pi l_t \frac{9(1-\nu)}{2t_c} \frac{l_c - \frac{1}{2} l_p}{l_c} (\Delta\sigma_1 - \Delta\sigma_2) \end{aligned}$$

Where l_p and t_p are the length and thickness of the piezo-resistor, respectively. Since the geometric variables x and z are linear in equation, the resistance change of the piezo-resistor is merely the result of that equation evaluated at the center of the piezo-resistor. Figure shows the results from this analytical solution compared to the FE model calculated from either the complete formulation as given in equation or the simplified formulation using the stress difference as given in equation. It can be seen that the first analytical model overestimates the solution by at least 35%. This is due to the incapacity of the model to correctly describe the distribution of the stress in y -direction close to the cantilever base as previously discussed and shown in Fig 2. If the piezo-resistor is placed very close to the clamped end, a better approximation is achieved by assuming zero stress in y -direction, thus taking out the factor of $(1 + \nu_c)$ in equations. The resulting change is shown in Figure and it is given by

$$\Delta\sigma_h(x, z) = \sigma_x - \sigma_y = (1 + \nu_c)\sigma_x = \frac{F \cdot 12 \cdot (1 + \nu_c)}{w_c t_c^3} (l_c - x)z$$

The deviation of the FEM solutions from the linear behavior is caused by geometric non-linearities at large tip deflections ($47.0 \mu m$ at $500 \mu N$), which are accounted for in this type of analysis. The fact that the two FEM solutions differ by no more than 5.3% indicates that the stress difference $\Delta\sigma_h$ as defined in equation is indeed a good measure for the piezoresistive response. Therefore, this parameter will be used in most cases throughout this work. In real cantilever devices, the density of the dopants varies gradually along the cantilever thickness direction, which is due to the micro fabrication processes and natural diffusion. This dopant distribution impacts both the piezoresistive coefficients and the resistivity, so that the exact solution cannot be described by an analytical expression. It is also difficult to measure the dopant distribution within the silicon, but the results of dopant implantation and heat treatment processes can be predicted well with simulation tools. When a dopant profile that approximates

a step function is achieved, equation can be a good estimate. Often, a fitting parameter β that accounts for the thickness and the dopant profile of the piezo-resistors is used. Its value ranges from zero (even doping throughout the cantilever thickness) to 1 dopants only at the top surface and concentration ideal for maximum sensitivity. Instead of using equation, the resistance change is then given by

$$\sigma_x(x, z) = \frac{F \cdot 12}{w_c t_c^3} (l_c - x)z$$

III. ANALYTICAL MODELLING OF PIEZORESISTIVE SURFACE STRESS SENSING CANTILEVERS

FEM was momentarily familiarized as a method to improve the results obtained from analytical formulae at the cantilever free end in the case of a point load. For the analysis of cantilevers that experience a surface stress, FEM is more important. Therefore, a more detailed description about the methods used in this work will be given in this section. All of the FEM simulations were done using the software package COMSOL Multiphysics 4.2a. To apply a surface stress on the top side of the cantilever, a layer of three-dimensional or two-dimensional elements is simulated that is pre-stressed with some given stress value. If the equivalent surface stress on the cantilever is the input variable to the FE model, the latter case is more efficient since two-dimensional elements require less computing power and the results are more accurate. All of the preferred element types are of high order, which gives more accurate results at a given mesh density and permits for the calculation of large, non-linear deformations. The film thickness has to be multiplied as shown in equation in order to calculate the surface stress caused by this virtual (2D) or realistic (3D) layer, and the unit of the resulting surface stress will be force/length. For all FE simulations in this work, the μ MKS system of units is employed, in which the units for length, mass, time, force, stress (pressure), and surface stress are 1 μ m, 1 kg, 1 sec, 1 μ N, 1 MPa, and 1 N/m, respectively. These units are very convenient for MEMS because the typical length scale is on the order of 1-100 μ m, and the typical stress levels are on the order of 1-100 MPa. Instead of just constraining one of the cantilever ends directly, part of the anchoring silicon substrate is modelled in all calculations. This results in a more realistic stress distribution, especially at the cantilever base, i.e. the clamped end. Whenever possible, i.e. in all cases except for modal analyses, only one half of the cantilever is modelled and the cutting plane (along the cantilever length and thickness directions) is constrained with symmetry boundary conditions to reduce the computation time and required memory. The objective of the FE modelling is to find the stress distribution, especially the stress difference $\Delta\zeta_{lt}$, within the piezoresistive volume of the cantilever and to maximize this value by modifying the cantilever geometry as well as the piezoresistor geometry and placement.

$$\Delta R/R = \beta \pi_{lt} \frac{6}{w_c t_c^2} \left(l_c - \frac{1}{2} l_p \right) F$$

With the definition of the spring constant for a rectangular cantilever the resistance changes due to a point force, equation, can be converted into the resistance change due to a free end deflection by

$$\Delta R/R = \beta \pi_{lt} \frac{3E_c t_c}{2l_c^3} \left(l_c - \frac{1}{2} l_p \right) \delta$$

If the stress state inside the cantilever for the case of a surface stress is assumed to be similar to that of a point load case, equation can be combined with the equations from previous sections to determine the resistance change due to surface stress.

$$\begin{aligned} \Delta R/R &= \pi_{lt} \frac{1}{l_p t_p} \int_0^{l_p} \int_{\frac{t_c}{2t_p}}^{\frac{t_c}{2}} \frac{F \cdot 12 \cdot (1 + \nu_c)}{w_c t_c^3} (l_c - x) z dz dx \\ &= \pi_{lt} \frac{12(1 + \nu_c)}{w_c t_c^3} \left(l_c - \frac{1}{2} l_p \right) \left(\frac{t_c}{2} - \frac{t_p}{2} \right) F \end{aligned}$$

IV. DESIGN OF PIEZORESISTIVE SURFACE STRESS SENSING CANTILEVERS

The stress distribution in a cantilever with surface stress is similar to that of a cantilever with a given tip deflection. The most viable approach to explore the validity of this assumption, is to look at the stress distribution in the cantilever at its top surface. The Figure compares the stresses in x- and y-directions, σ_x and σ_y , for the case of a cantilever with point load and a cantilever with surface stress. The loading levels are chosen, such that the piezoresistive change from equations should be identical.

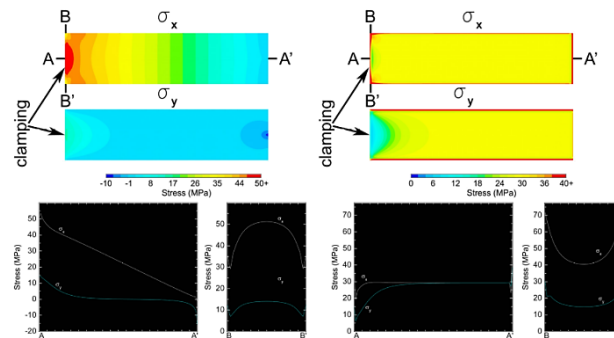
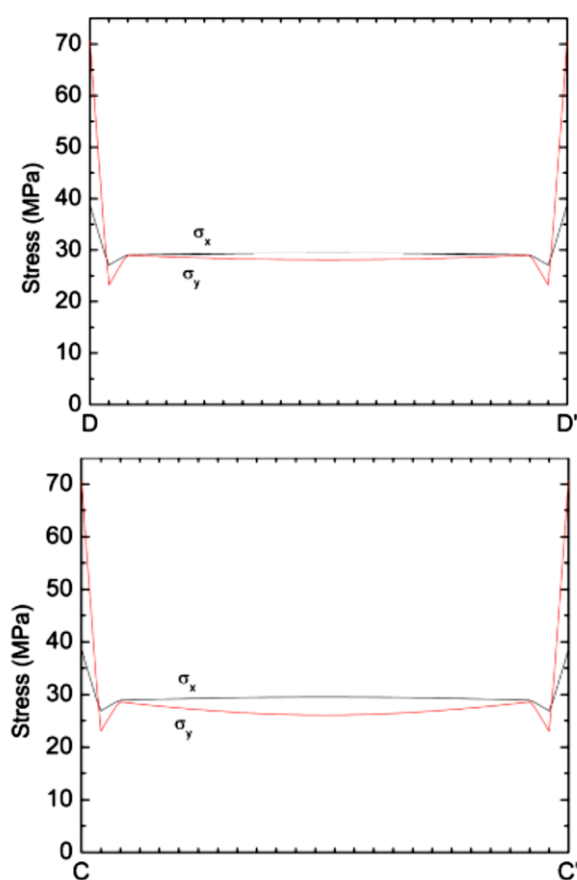


Fig.3 Stress distributions within the cantilever and thus the piezoresistive output signal

The two loading cases comparison clearly displays that the stress distributions within the cantilever and thus the piezoresistive output signal are very dissimilar. While the point force causes a stress distribution with a linearly decreasing stress in x-direction and a stress of much smaller magnitude in y-direction, this is not the case for the cantilever surface stress loading.

In the latter case, if the plate is not constricted the surface stress causes isotropic bending in all directions so both stresses are equal far away from the clamped base. The stress in x-direction ranges the value equivalent to the stress in a free plate far closer to the base than the stress in y-direction as shown in bottom section of Figure. The reason is that since the width is much

greater than the thickness, the clamping of the cantilever along its width is much more constricting for bending in the y-direction. One instantaneous design consideration based on these results is the variation of the cantilever width to modify the amount to which the stress in y-direction is restricted at the base. This will be conversed later in this section. It has been shown that the piezo-resistor should be placed close to the cantilever base for greater sensitivity. In this framework, the question arises that the placement in y-direction is important or not. Figure seems to indicate that the stress difference is higher at a local stress concentration point on the outside of the cantilever than in the cantilever center. Therefore, it seems as though this would be the ideal placement for the piezoresistive element. However, Figure indicates that the stress difference decreases much faster along the cantilever edges than at the center.



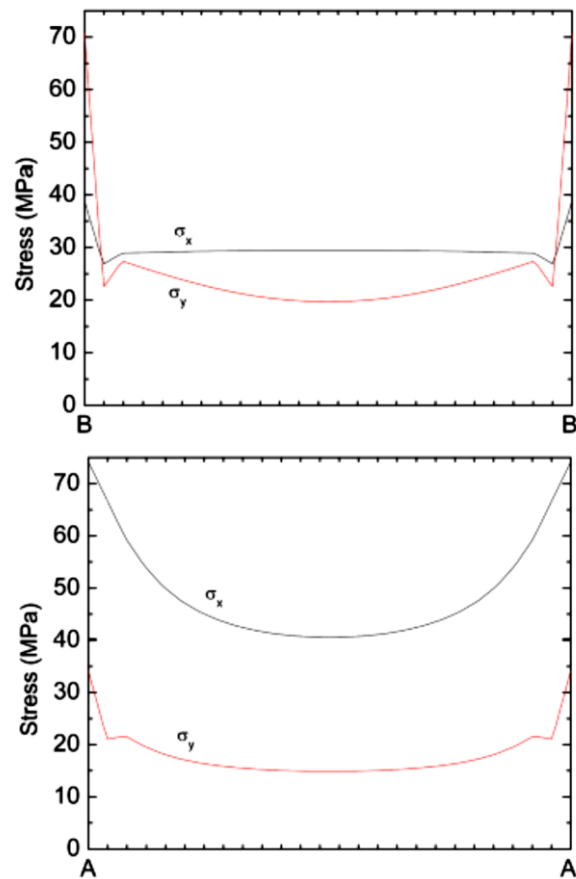


Fig.4 Stress distribution across cantilever

Since the piezoresistor must always be of certain minimum dimensions set by the fabrication process, placing the piezoresistor on the cantilever edge would result in a reduced sensitivity. The high spike at the very edge within each cross-section is yet another effect, which is very much localized at the edge and results from the singularity at the unconstrained side wall. Most micro fabrication processes for microcantilevers involve a process step in which the wafer is etched through from the backside to release the free hanging devices. This requires the alignment of the photo mask on the wafer backside to the features on the front side of the wafer, as well as a long etch process. Both of these steps have an inherent uncertainty for the location at which the backside trench will meet the cantilever devices. Therefore, it is necessary to make the piezoresistors of a certain minimum length, so that at least the largest part of the piezoresistor at the cantilever base is within the free-hanging area of the cantilever. Furthermore, for a given piezoresistor length, there is also a minimum width so that the resistance of the sensing area can be kept within given design criteria. Here, it will be assumed that the minimum length and width for the piezoresistive area are each on the order of 40-60 μm for the employed micro fabrication process. For a given piezoresistor placement and size, the shape of the cantilever can be reformed to improve the piezoresistive signal due to a surface stress on the cantilever. The stress difference $\Delta\sigma_{lt}$ within the top third of a cantilever of 200 μm length, 50 μm width and 1 μm thickness, and loaded with a surface stress is shown in Figure 3.7a. These dimensions are realistic for devices that have been used for chemical sensing in previous studies. The piezoresistive area of 40 x 40 μm^2 at the center of the cantilever base is

shown as a dashed line in the figure. It can be seen that the stress difference $\Delta\sigma_{lt}$ which is a measure for the piezoresistive output signal, is zero for all areas except close to the clamping. It can also be seen that the stress state in this region does not vary significantly for cantilevers of the same width, thickness and surface stress loading when the length is changed to 100 μm , 50 μm , and 400 μm as shown in Figure. The average $\Delta\sigma_{lt}$ for the region marked with the dashed line in these figures is plotted thickness (t) vs. the cantilever length (l) in Figure is shown.

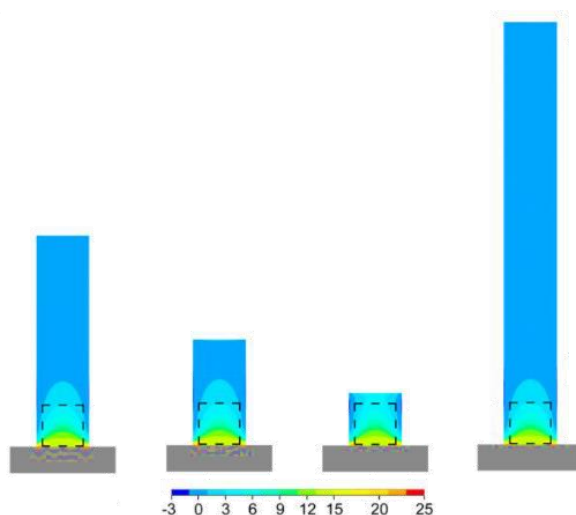


Fig: stress state of cantilevers of the same width, thickness and surface stress loading when the length is changed to 200 μm , 100 μm , 50 μm , and 400 μm

In comparison to the case with a point force at the cantilever free end, it can be observed that, the length of the cantilever does not affect the piezoresistive output signal ominously in the case of a constant surface stress. If the piezoresistive signal and thus the sensitivity cannot be improved by making the cantilever longer, it is interesting to investigate whether this effect can be achieved by increasing the cantilever width. In the previous discussion, it was supposed that a wider cantilever will be more resistive to bending in the width direction while the clamping has little influence on the stresses along the length direction. Therefore, keeping both the length and the surface stress loading as constant, the stress difference $\Delta\sigma_{lt}$ should be higher for wider cantilevers. The stress differences $\Delta\sigma_{lt}$ in the top third of cantilevers with identical surface stress loading, a length of 200 μm and widths of 50 μm , 100 μm , 200 μm , and 400 μm are shown in Figures respectively. It can be seen that the magnitude of $\Delta\sigma_{lt}$ with the cantilever width. Furthermore, for wider cantilevers, the high stress values are present in larger parts of the previously defined piezoresistive area marked with dashed lines in the figure.

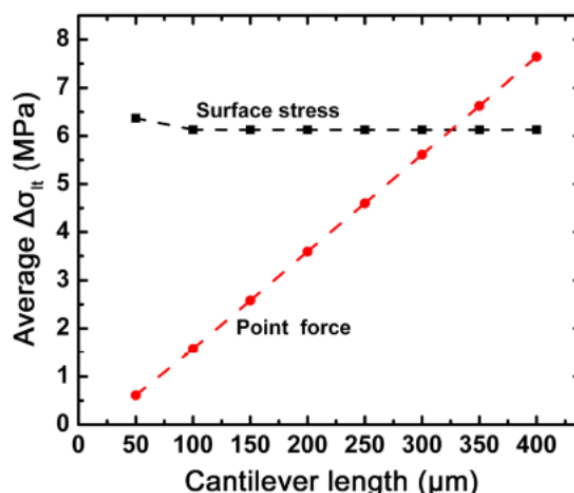


Fig.5 Cantilever length in μm vs Average $\Delta\sigma_{lt}$

Therefore, the average $\Delta\sigma_{lt}$ increases and subsequently the sensitivity to surface stress loading increase with the cantilever width. This is shown in Figure compared to the case for a point force at the free end, for which the sensitivity decreases with increasing width as estimated from theory. It can be seen that for the given piezoresistor shape and cantilever length, the cantilever width should be at least $150\ \mu\text{m}$ to be in the regime to the right of the steep increase in the sensitivity. In this regime, the sensitivity only increases moderately with cantilever width, so that there is a tradeoff between slightly improved sensitivity and greatly worsened compactness of the cantilever. An extremely wide cantilever is also unfavorable for the design and fabrication process as it requires a large space along the substrate and a backside etch process that is uniform enough to reach the right edge position at all points along the cantilever width. From these considerations, it can be concluded that a cantilever with width $200\ \mu\text{m}$, i.e. an length to width ratio of one, is a good compromise between sensitivity and compactness for the given piezoresistive area and cantilever length.

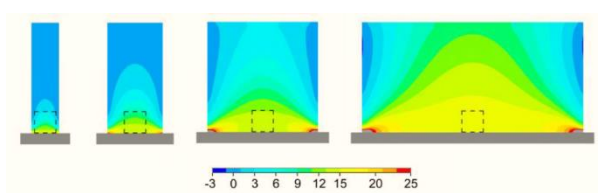


Fig.6 stress state of cantilevers

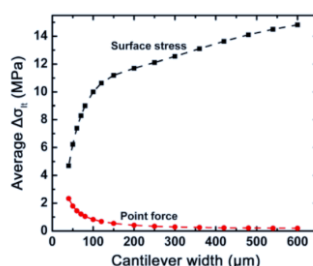


Fig.7 Cantilever length in μm vs Average $\Delta\sigma_{lt}$

It is fascinating to see what effect the cantilever area has on the sensitivity if the ratio of cantilever length to width and the piezoresistive area both are fixed. The average stress difference $\Delta\sigma_{lt}$ is conspired as a function of the cantilever area for the defined scenario in Figure. It can be observed in this case about that an increase in the area beyond a certain value, does not lead to an increase in sensitivity.

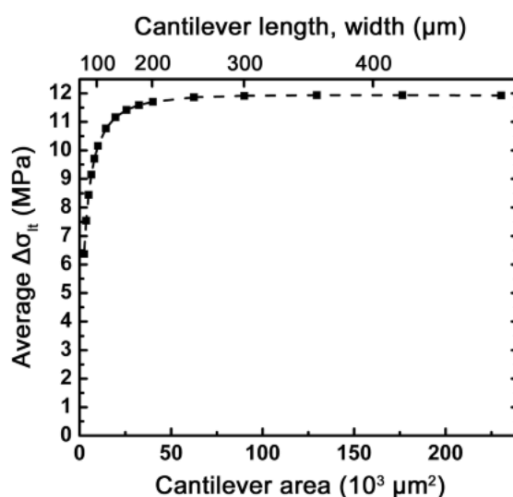


Fig.8 Cantilever length in μm vs Average $\Delta\sigma_{lt}$

The figure also shows that increasing the cantilever length is actually counterproductive as the sensitivity does not extent the same values as in Figure above for large widths. The cantilever thickness is another important parameter for the sensitivity to surface stress. As the cantilever stiffness increases with its thickness, thin cantilevers should be advantageous. In the case of a given point force at the free end, from equation. it can be seen that the maximum value for $\Delta\sigma_{lt}$ (at $z=lc/2$) is proportional to the square of the cantilever thickness. However, in practical applications where the piezoresistor thickness is determined by the fabrication process, reducing the thickness is not always beneficial. In these cases, the centerline of the piezoresistor is moved closer to the neutral axis of the cantilever as the cantilever thickness is decreased resulting in a decrease in sensitivity. The piezoresistive signal is shown as a function of the cantilever thickness for the case of a surface stress loading, in Figure 3.10. The length and width dimensions of the explored cantilever are $200 \mu m$ each and the piezoresistive area is $40 \mu m$ square.

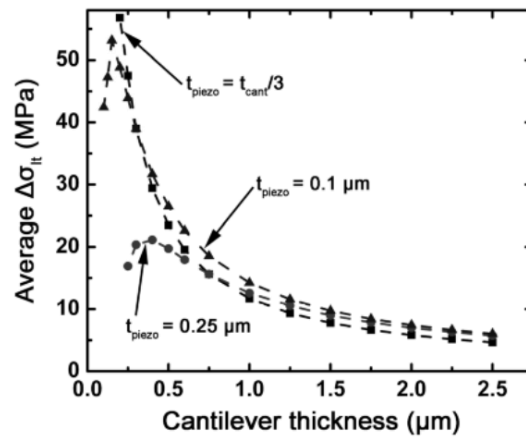


Fig.9 Cantilever length in μm vs Average $\Delta\sigma_{lt}$

The figure compares the cases of fixed piezoresistor thicknesses of $0.1\ \mu\text{m}$ and $0.25\ \mu\text{m}$ and the one in which the piezoresistor thickness is one third of the cantilever thickness. For the latter case, with decrease in cantilever thickness the output signal increases as expected. The relationship can be estimated well as inversely proportional. For the cases in which the piezoresistor thickness is fixed, the sensitivity at first also increases with decreasing cantilever thickness. Yet, because of the piezoresistors proximity to the neutral axis when the cantilever thickness gets below a certain value the signal decreases. However, as opposed to the point load case, the signal does not go to zero when the piezoresistor thickness is equal to the cantilever thickness. There are two reasons for this effect. Firstly, the stress distribution is a strong function of the position in cantilever width direction and the signal is only determined by a portion of the width. Secondly, due to the surface stress boundary condition, the beam does not have a free top surface, and thus the beam equations within the cantilever do not have to be fulfilled. This means that the result from integrating the stress in cantilever length direction over the cantilever thickness does not have to be zero. The maximum sensitivity for the given scenario is achieved when the piezoresistor thickness is about two thirds of the cantilever thickness. Furthermore, the cantilever thickness should be minimized to maximize the sensitivity.

V. CONCLUSION

Finally it can be concluded that the cantilever width and thickness as well as the dimensions of the piezoresistor are the dominant parameters for the sensitivity to surface stress. The piezoresistor should be placed in the center of the clamped base, and it is always advantageous to minimize the piezoresistor length, width and thickness to achieve higher sensitivity. However, due to fabrication processes, such as etch uniformity, and design restrictions, such as maximum total resistance, these parameters regularly have lower limits. For a piezoresistor of finite dimensions, the sensitivity increases with increasing cantilever width, whereas the cantilever length has little effect on the sensitivity. Reducing the cantilever thickness increases the sensitivity until a maximum is reached when the cantilever thickness is about one and a half times the piezoresistor thickness.

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