Optimization of Micromachined Photon Devices

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ABSTRACT

The Oak Ridge National Laboratory has been instrumental in developing ultraprecision technologies for the fabrication of optical devices. We are currently extending our ultraprecision capabilities to the design, fabrication, and testing of micro-optics and MEMS devices. Techniques have been developed in our lab for fabricating micro-devices using single point diamond turning and ion milling. The devices we fabricated can be used in micro-scale interferometry, micro-positioners, micro-mirrors, and chemical sensors. In this paper, we focus on the optimization of microstructure performance using finite element analysis and the experimental validation of those results. We also discuss the fabrication of such structures and the optical testing of the devices. The performance is simulated using finite element analysis to optimize geometric and material parameters. The parameters we studied include bimaterial coating thickness effects; device length, width, and thickness effects, as well as changes in the geometry itself. This optimization results in increased sensitivity of these structures to absorbed incoming energy, which is important for photon detection or micro-mirror actuation. We have investigated and tested multiple geometries. The devices were fabricated using focused ion beam milling, and their response was measured using a chopped photon source and laser triangulation techniques. Our results are presented and discussed.

Keywords: MEMS, microcantilever, finite element analysis, FEA

1. INTRODUCTION

The desire to shrink the size of mechanical components, optical devices, and sensors to sizes obtained by the microelectronics industry has driven a significant amount of research in the field of micro-electro-mechanical systems (MEMS).¹ Micromechanical devices are currently being considered for a wide variety of applications including uncooled infrared detectors, micro-actuators, chemical detectors, and completed mechanical systems. Currently the dominant manufacturing method for micro-devices is the microlithography approach used by the microelectronics industry.² This approach works well for producing a large quantity of devices, however the ability to produce prototype devices is not as developed as the ability to mass-produce devices. The ability to simulate the response of micro-devices using finite element analysis (FEA) gives researchers insight into the behavior of devices before prototypes are developed or production runs occur as well as allowing the designer to optimize the desired response.

Photon detectors^{3,4} represent a class of MEMS devices which have been studied with great interest.⁵ Several different types of photon detectors are available including CCDs, microbolometers, thermopiles and pyroelectrics.^{5,6} Solid state infrared detectors must be operated at reduced temperatures from the ambient in order to reduce thermal noise.⁷ The infrared thermal detectors discussed here convert the incident radiation into heat which produces a change in the position of the micro-cantilever through bimetallic bending or other effects.^{14,8} The goal of this research is to study the effects of several design variables on the bending of microcantilever structures.

Figure 1: Image of folded-leg thermal detector or cantilever.

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For this experiment, a “folded-leg” thermal detector was fabricated using focused ion beam milling.’ The goal in the design of this device was to create a compact, sensitive, thermal detector. A large collecting area was defined at the end of a folded leg structure to maximize the energy absorbed. The purpose of folding the legs five times was to create a compact device that behaved thermally and mechanically as a larger device. The device with the legs folded five times as shown in Figure 1 is referred to as a **pentalever**. The collecting area **is** also the area used for optically measuring the displacement.

2. FINITE ELEMENT MODELING

2.1 Finite Element Analysis

The concept of **structural finite** element analysis involves obtaining an approximate solution for the displacement values of a continuum by dividing that continuum into a number of ‘finite elements’ and solving the function representing the displacement of those nodal points. Often the energy required to displace the nodes, or strain energy is used to solve the equations. These elements are connected at a specific number of nodal points on their boundary. Functions are chosen to represent the displacement within the **finite** element based on the nodal displacements. The displacement functions **can** be used to determine the state of strain within the finite element as a function of the nodal displacements. The knowledge of these strains combined with any existing internal strains and the elastic properties can be used to determine the state of stress within **the** elements. Existing internal strains would be the result of thermal expansion or other similar phenomena. A system of forces is applied at the nodal points which is equal to any distributed loads or applied boundary stresses such that the system is in equilibrium. The element displacement in terms of the applied and internal forces is given by the following equation:

$$\{F\}_a = [k]_a \{\delta\}_a + \{F\}_{a,p} + \{F\}_{a,sw} \quad (1)$$

where $\{F\}_a$ is the matrix representing the force vectors at all of the nodes of an element ‘a’, $\{F\}_{a,p}$ is the force matrix resulting from applied nodal forces or distributed loads, $\{F\}_{a,sw}$ represents forces on the nodes resulting from internal strains, The matrix, $[k]$, is the element stiffness matrix, and $\{\delta\}_a$ represents the **displacements**.⁹

The finite element modeling package **Pro/Mechanica** was utilized to develop the model for our devices. **Pro/Mechanica** was chosen for it’s high degree of automation in performing optimization studies, and because it uses “geometric” elements. Geometric elements are also **referred** to as polynomial or ‘p’ type elements. Although this structure did not take advantage of the p-element’s ability to exactly map curved surfaces, we did take advantage of the adaptive meshing and convergence checking ability of the p-element. The ability of the p-element to **perform** automated geometry optimization was utilized, whereby it would be more time consuming to mesh the **geometry** during each iteration of optimization.

Designers using finite element analysis are often concerned with discretization errors, or errors associated by modeling a continuous body by a series of finite elements. Conventional (h-method) finite element codes rely on dividing the structure into a **fixed** number of elements and solving the matrices associated with those elements and their boundary conditions. Upon solving the matrices associated with the model, the finite element mesh associated with that model is refined by subdividing the elements. Results of each analysis are compared to the previous analysis until the results agree to within a certain percentage. More recently, p-method finite element codes have been introduced which make use of high-ordered polynomial elements. P-element convergence is achieved by increasing the polynomial order of the individual elements. In order to save computational resources the algorithm used by **Pro/Mechanica** checks the individual elements for convergence **and** only increases the polynomial order of the elements that have not converged. This type of analysis allows convergence to be checked and accuracy ensured without the need to completely recreate the element mesh. The p-method of finite element analysis was developed in the early 1980’s with significant contributions in the literature by I. Babuska, B. Szabo, and A. Peano, and others.”

The displacement and rotation **field** variables are given in terms of a polynomial series:

$$u = \sum_{i=1}^n \begin{bmatrix} u_x^{(i)} \\ u_y^{(i)} \\ u_z^{(i)} \end{bmatrix} l^{(i)} \quad \beta = \sum_{i=1}^n \begin{bmatrix} \beta_x^{(i)} \\ \beta_y^{(i)} \\ \beta_z^{(i)} \end{bmatrix} l^{(i)} \quad (2)$$

where $\mathbf{u}$ is the displacement vector and β is the rotation vector. The functions, $\mathbf{t}$, are the hierarchical polynomial basis functions given by Babuska, Szabo, and Katz.^{11,12}

Figure 2: Finite element geometry of micro-device structure.

2.2. FEA Procedure

The FEA model of the micro-device was developed in Pro/Mechanica consisting of 804 two-dimensional shell elements and 1,120 three-dimensional solid elements. The 804 two-dimensional shell elements were used to represent a thin layer of gold on the top of the triangular-shaped cantilever, and the solid elements were used to represent the silicon material in the triangular shaped cantilever and heat sink. The gold layer had a nominal thickness of 50 nanometers, and the cantilever itself had a thickness of 1 micrometer. The base of the triangular shaped cantilever was 200 micrometers and the height was 160 micrometers. The microstructure consists of a large absorbing area near the tip. The legs of the cantilever are folded five times before they attach to the heat sink in order to increase the thermal resistance of the system.

A steady-state analysis was performed on the model using conditions similar to those seen during laboratory experiments with a similar structure. A heat load was applied to the surface of the cantilever equivalent to $0.1\mu\text{W}$. The starting temperature of the structure was set to be 0°C in order to reduce any errors due to round-off or division by very small numbers. Setting the starting temperature at 0°C also allows the results to represent the change in temperature. The heat loads were used in a thermal analysis to calculate the deflections caused by the incident, radiant energy. The temperature changes were transferred to the structural analysis and used to calculate the thermal deflection.

A modal analysis was performed to calculate the first four fundamental frequencies of the micro-device. Results of this analysis are used to gain insight into the potential response of the device. Convergence of 10 percent was achieved on all results.

An optimization study was performed to determine the effects of the bimaterial coating thickness on the maximum temperature change and the maximum deflection. In the optimization study, the thickness of the gold coating was varied from 50nm to 500nm. The analysis was performed to determine the effect of thickness on the maximum temperature change in the cantilever surface and the effect of coating thickness on the maximum temperature obtained by the cantilever. The $200\mu\text{m}$ wide by $160\mu\text{m}$ long cantilever was attached to a silicon "heat sink" that was $500\mu\text{m}$ wide, $200\mu\text{m}$ thick, and $200\mu\text{m}$ deep. The bottom surface of the heat sink was constrained thermally to be 0°C and was constrained structurally from all displacements.

To further improve thermal sensitivity, a change was made in the way the coating was simulated. Instead of simulating the entire top surface of the detector as having a gold coating, the coating was applied to the top of the first, third, and fifth folds of the legs, as well as the entire top of the collecting surface. The coating was then applied to the bottom surfaces of the second and fourth folds of the legs, as well as the entire bottom surface of the collecting area. The coating was simulated on both sides of the collecting surface in order to minimize the distortions in this surface. Distortions in the collecting surface result in an optical power or "lensing effect" and make optical measurement of deflections more difficult,

2.3 Micro-cantilever Thermal Detector

The selection of the infrared (IR) thermal detector plays an important role in the ultimate system sensitivity. Presently, there are a number of families of commercially available IR detectors, including thermopiles, bolometers, pyroelectrics, and various solid state detectors.^{2-7,13-15} In this work, we employed inexpensive micromechanical IR thermal detectors, which are based on the bending of a microcantilever as a result of absorption of IR energy.^{8,14-20} When a microcantilever is exposed to IR radiation, its temperature rises due to absorption of this energy.

Bimaterial microcantilevers are constructed from materials exhibiting dissimilar thermal expansion properties. For example, microcantilevers made from silicon nitride (or silicon) coated with a thin film of gold or platinum will exhibit the bimaterial effect. The bimaterial effect causes the microcantilever to bend in response to temperature variations. The extent of bending is directly proportional to the radiation intensity. Previous work has shown that **microcantilever** bending can be detected with extremely high **sensitivity**.^{8,14-20} For example, metal-coated microcantilevers that are commonly employed in atomic force microscopy (AFM) allow sub-Angstrom ($< 10^{-10}$ m) sensitivity to be routinely obtained. Recent studies have **reported**¹⁷⁻²⁰ the use of **microcantilever** bending for calorimetric detection of chemical reactions with energies as low as a few pJ. It was demonstrated*⁷ that a similar microcantilever thermal detector had an observed sensitivity of 100 pW corresponding to an energy of 150 fJ and use of the sensor as a **femtojoule** calorimeter was proposed. An estimate of the minimum detectable power level was on the order of 10 pW, corresponding to a detectable energy of 10 fJ and a temperature sensitivity 10^{-5} K. However, using an optimally designed microcantilever, the sensitivity may be improved even further.

The bending of a rectangular bimaterial microcantilever is proportional to the absorbed energy. The maximum deflection, $z_{\max}$, due to differential stress is given by “,”

$$z_{\max} = \frac{5}{4} \frac{(t_1 + t_2)^3}{(\kappa_1 t_1 + \kappa_2 t_2) w t_2^2} \times \frac{(\alpha_1 - \alpha_2)}{4 + 6 \frac{t_1}{t_2} + 6 \frac{t_1^2}{t_2^2} + \frac{E_1 t_1^3}{E_2 t_2^3} + \frac{E_2 t_2}{E_1 t_1}} \times \eta \left(\frac{dQ}{dt} \right) \quad (3)$$

where l and w are, the length and width of the microcantilever, respectively, t_1 and t_2 are the thickness of the two layers, κ_1 , κ_2 , α_1 , α_2 , E_1 , E_2 are the thermal conductivities; thermal expansion coefficients, and modulus of elasticity of the two layers, and $\eta dQ/dt$ is the fraction of the IR radiation power absorbed. In order to increase the IR detection sensitivity of a microcantilever, $z_{\max}$ should be maximized. Note that $z_{\max}$ is strongly dependent on the geometry and thermal properties of the two layers.

3. EXPERIMENTAL

We investigated the response of our devices using the experimental setup shown in Figure 3. To detect movement of the cantilever, a diode laser (delivering 1 mW at 670nm) was focused on the tip of the microcantilever using a 20-power microscope objective. In order to minimize heating of the tip by the probe laser, optical power was reduced by placing a neutral density filter with an optical density of 1.0 between the probe laser and the objective. A quad-element (A,B,C,D) photodiode detector was used to collect the reflected probe beam. The current output ($i_{A,B,C,D}$) of the photodiode depends linearly on the bending of the microcantilever. A high, narrow bandpass optical filter was placed in front of the photodiode allowing the laser beam to be detected while preventing other wavelengths from reaching the photodiode. The amplified differential current signal from the quad cell photodiode, $i_{A,B,C,D} [(i_A + i_B) - (i_C + i_D) / (i_A + i_B + i_C + i_D)]$, was monitored and recorded using a digital oscilloscope (TDS 780, Tektronix) or sent to a lock-in amplifier (SR850, Stanford Research Systems) for signal extraction and averaging.

Figure 3: Schematic diagram of experimental setup

The cantilevers used for this experiment were triangular silicon **pentalevers** and two different designs were studied. The first design was 1.0 μm thick and had a 50 nm thick gold/chromium film uniformly covering one side. A **modified** version of the first design was studied which was 1 μm thick and had the gold coating applied to the entire front and back surface of the detector “pad” area and alternated on the front and back of the folded legs. Optical read-out was used to measure the bending of the microcantilever thermal detector. Since the quad element photodiode was blind to IR, no additional filtering **was** needed for the read-out circuit.

4. RESULTS

4.1. Modeling Results

Modal analysis was performed to determine the first four fundamental frequencies of the device. The results of the modal analysis are shown in Table 1. The mode shape for the fundamental frequency is shown in Figure 4. The analysis of the mode shapes gives insight into the potential dynamic response of the device, as well as the potential motion of the device during excitation.

Table 1: Micro-device natural frequencies.

Mode	Frequency (kHz)
1	12.72
2	41.23
3	47.41
4	84.88

The thermal response of the cantilever to the $1\mu\text{W}$ heat load is shown by the temperature distribution in Figure 5. The energy flow from the pad area at the tip through the folded leg geometry is apparent. The temperature change along the path goes from greater than 0.2°C to less than 0.02°C as the thermal energy flows from the pad area to the heat sink. The maximum temperature change in the model when subjected to the $1\mu\text{W}$ heat load was 0.23°C . Figure 6 shows the thermal bending of the folded leg cantilever. The maximum displacement due to bimetallic bending was 1.86 nm.

Optimization studies were performed to predict the tip displacement of the cantilever as a function of energy and to determine the effects of increasing the coating thickness on the displacement of the cantilever. Our results show that the effect of energy on the displacement of the cantilever tip were linear.

Increasing the coating thickness resulted in a decrease in the maximum temperature change achieved in the cantilever. Due to an increase in the bimetallic effect with increased coating thickness, the bending increased to a maximum and then dropped off. The decrease in bending at the greatest coating thickness was due to the overall decrease in thermal resistance. The results of the optimization study are shown in Figure 8, which plots maximum deflection and maximum temperature as a function of coating thickness.

A steady-state thermal analysis was performed on the cantilever model with the simulated coating applied to alternating legs and both sides of the sensing pad area. For the $1\mu\text{W}$ heat load the alternating coating geometry experienced a maximum displacement 7.91 nm as opposed to 1.86 nm for the original geometry. These results agree well with preliminary experimental results that show a factor of three improvement in response by alternating the coating. Due to the larger gold-coated area on the alternating coating geometry, the maximum temperature change was 0.226°C as opposed to 0.265°C for the original geometry

Figure 4: Mode shape of the fundamental frequency.

Figure 5: Temperature results from the $1\mu\text{W}$ energy load. ΔT in degrees Centigrade.

Figure 6: Exaggerated micro-device displacement due to bimetallic bending in mm. Coating only simulated on the top surface.

Figure 7: Simulated displacement of pentalever with alternating bimaterial coating on the top and bottom of legs.

Another interesting effect of alternating the coating on the folded leg geometry and coating both sides of the collecting area was that more of a pure rotation of the collector area occurred. The rotation of elements in the center of the collector area was 0.0041" compared to 0.0013" for the device coated entirely on the front surface. The difference in the amount of warping of the collector surface is seen by comparing Figures 6 and 7.

4.2. Thermal Detector Measurements

In order to optimize the thermal detectors used in our micro-spectroscopy techniques, we investigated the response of microcantilevers to IR radiation. A HeNe laser was used to thermally excite gold-coated microcantilevers. The bending of the microcantilever was determined using an optical read-out scheme as described earlier. The signal was digitized and stored, or sent to a lock-in amplifier. Assuming a uniform heat dissipation over the entire length, l , of the microcantilever (of thickness t) the change in temperature at the tip, ΔT ($\approx l^2/2\lambda dQ/dt$), depends on geometry factors such as l and t . A temperature change of $\Delta T=10^{-4}$ K leads to deflections of approximately 1 nm.

Assuming a spatially uniform incident power, dQ/dt , onto a bimaterial microcantilever, the maximum deflection depends on the temperature rise^{6,14,17} and is proportional to the incident power.^{14,17} The thermally induced deflection of the microcantilever is caused by the bimaterial effect which arises due to the difference in the thermal properties of the metal layer and the geometry of the microcantilever. In Figure 10, we plotted the maximum bending, $z_{\max}$, as a

Figure 8: Coating thickness optimization study results. Displacement and maximum temperature change as a function of coating thickness.

function of the absorbed power, P_{th} , and it can be seen that the **maximum** bending increases linearly with increasing power. The reflectivity of the gold film is >0.99 , and the reflectivity was taken into account when determining the absorbed power. From the slope of the line in Figure 10, we obtained a deflection sensitivity of approximately 0.053 nm/nW . Using a Stanford Research Systems SR 540 chopper to modulate the IR radiation at a **frequency** of 30 Hz, we calculated a noise equivalent power (NEP) of $520 \text{ pW/Hz}^{1/2}$.

The micro-cantilever thermal detector was found to exhibit two distinct **thermal** response times due to the incoming IR radiation; a time $\tau_{th,1} < 1 \text{ ms}$ and a time $\tau_{th,2}$ that is somewhat longer ($\sim 10 \text{ ms}$). The fast thermal response is attributed to thermal equilibrium between the top (exposed to the IR radiation) and the bottom surfaces, while the longer thermal response results from the heat flow (along the body of the microcantilever) to the supporting base.

Since the read-out scheme employs laser beam reflection from the microstructure pad, the alternating bimaterial approach has **an** additional advantage over previous configurations. Since the device pad is metal coated from both sides, there is only a deflection in the supporting leg structure. In previous approaches the pad would also warp from the bimaterial construction and cause a **lensing** effect. This effect provided some measurement difficulties since it was necessary to compensate for probe beam convergence or divergence. We found nearly a factor of **three** improvement in response sensitivity for the alternating bimaterial pentalever structure compared to the simple bimaterial pentalever. The experimental results for both of these geometries are shown in Figure 9. Future direction for achieving greater sensitivity will focus on both material and **micromechanical** optimizations. The bimaterial effect can be further optimized by selecting polymers instead of metals to work with the silicon substrates. Certain **polymers** have a factor of four **greater** coefficients of expansion compared to even zinc. The micro-mechanical structure can be taken to the next logical level to produce a seven legged heptalever device.

5. DISCUSSION

The results of the finite element analysis can be used to gain insight into the behavior of the micro-device, and its response to the applied stimulus. The results of the modal analysis can be used to give insight into the expected shape of the device response and an approximation of the responsivity of the device to external stimulus. Figure 4 shows the shape of the device in response to the fundamental frequency. This represents the normal bending of the device expected and occurs at a frequency of 12.72 kHz as shown in Table 1. The other modes of the device represent vibrations of the individual legs of the device. Figure 5 shows the temperature distribution from the thermal analysis. In this figure, it was observed that the

Figure 9: Detector voltage for alternating coating pentalever (a) and top bimaterial coated cantilever(b). FEA results for a are shown in Figure 6 and b is shown in Figure 5.

Figure 10: Experimental data and transient FEA analysis results.

greatest temperature was achieved in the “collector” area at the end of the device, and the temperature can be seen to decrease along the legs of the device indicating heat transfer through the legs of the device itself. Figure 6 illustrates the deformed shape of the cantilever due to bimetallic bending. In designing this device, it was anticipated that the thermal deflection would greatly increase as each individual section of the legs deflected, however the model does not show this to be the case. The effect of folding the legs allows the thermal resistance of the device to be increased due to decreased area and increased path length, which increases the deflection of the device due to bimetallic bending.

The results of the optimization study indicate that changing the coating thickness has a tremendous influence on the temperature change of the device and the maximum deflection. The optimum thickness is seen in the peak of the coating thickness versus maximum bending plot shown in Figure 8. It should be noted that the peak in the displacement versus coating thickness curve occurs due to several of the properties in the gold layer. Although the gold layer has a higher coefficient of thermal expansion than silicon, the gold layer also has a higher thermal conductivity. Therefore as the coating thickness is increased, a limit is reached where the increase in the transport of energy away from the detector negates any benefits from increased coating thickness.

Figure 10 compares the results of the transient analysis with the experimental results. The sensitivity of the pentalever was determined experimentally to be $0.0528 \text{ nm}/\mu\text{W}$ and determined to be $0.0838 \text{ nm}/\mu\text{W}$ by the analysis. These results are for the pentalever coated only on the top surface.

Boundary conditions are one of the most important considerations in any finite element analysis. It is very important to consider all loads, constraints, and accurately model the geometry. The area of MEMS metrology and material properties determination is a wide field unto itself.²¹⁻²³ The cantilever geometry was modeled as accurately as possible; however due to difficulty in measuring sub-micron features, some deviation in the actual geometry from that modeled is expected. Coating thickness deviations and internal stresses are other sources of error that are difficult to quantify. Due to these uncertainties, it was expected that the analysis would give an “order-of-magnitude” type of prediction. The results of the analysis agreed reasonably well with the experimental results.

The improvement in the response seen in the laboratory by alternating the coating was predicted by the finite element analysis. The amount of improvement seen in the lab was slightly less than that predicted, and that may be attributed to differences between the individual cantilevers tested. Direct comparison of these two geometries is difficult, due to the fact that the amount rotation and displacement of the non-alternating coating cantilever varies significantly along the length of the cantilever.

6. CONCLUSIONS

Finite element analysis has proven to be a powerful tool in designing micro-devices and structures. Simple changes in the geometry of micro-sensors can have significant effects on their response. In this paper, the effects of varying the bimaterial coating thickness were shown to have drastic effect on the response of the device. The analysis proved to be an effective tool in understanding the response of the system and gave tremendous insight into the direction for improvements. The initial analysis of the single-side coated cantilever gave insight as to the necessity to apply the coating to alternating legs of the pentalever. The analysis showed that the alternating coating would solve problems encountered by the “lensing” of the detector surface, provide a pure rotation as opposed to a curling of the detector surface, and deliver a factor of four better response. These results compared well with the factor of three increase in response seen in the lab.

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