Investigating the Coefficient of Thermal Expansion of PECVD TEOS SiO$_2$ on Silicon

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Abstract

The goal of the experiment was to determine the coefficient of thermal expansion for PECVD TEOS on SiO$_2$ on silicon using surface machined MEMS. Two different devices were used to investigate the property along with an available environmental chamber and an optical interferometer. One device yielded no results and the other device needs tuning to yield more accurate results. The investigation as a whole proved that the methodology works should devices be obtained or fabricated that could measure what is necessary to calculate the coefficients accurately.

Introduction

While the coefficient of thermal expansion (CTE) of silicon dioxide is known for bulk material (thick film), a coefficient for thin films (t ~ 2 μm) is relatively unknown. With the further development of Micro-Electro Mechanical System (MEMS), knowing this coefficient can help form devices made to operate at certain temperature levels predictably. Similarly, as devices are continuously being made smaller, knowing the dependence of film properties on dimension is required. In an ideal case, most modern electronic devices would operate at room temperature without gaining heat through operation. However, the laws of physics dictate that heat will be created through device operation, or perhaps the device operation actually involves a thermal stimulus (e.g. integrated heater for thermal actuation). Therefore knowing the thermal properties of a material will promote efficient designs. Some of the published thermal coefficients have been determined through local, resistive heating. This may not accurately portray the coefficient as the heating may not be even across the entire testing device. Global heating in an environmental chamber can provide uniform heating and a more reliable measurement.

Optical profilometry provides high-resolution surface measurements in 3D with sub-nanometer resolution in the vertical direction over a lateral range of millimeters. The Veeco Wyko NT1100 at RIT provides a quantitative determination of a variety of important material properties such as film thickness, surface roughness, and vertical and lateral dimensions of thin films and coatings. The primary advantage of this instrument over other metrology techniques is the flexibility to quantify each of these properties without physical contact. Enhancements to this system include a through-transmissive-media optical objective and an Analytical LTS350 environmental chamber probe stage from Linkam Scientific Instruments (see Figure 1) which provides precisely controlled temperature (-196 °C to 350 °C) and ambient conditions.

![Environmental chamber with 4" silicon substrate.](image1.png)

**Theory**

The first type of device that will be tested is shown in Figure 2 which is a vernier type structure. This structure has teeth on the end of the beam that will align to teeth on the opposing sidewall based on stresses in the film or thermal stresses. As parts of the beam expand or contract, the end should shift alignment and thus provide an accurate measure for approximately how much the beam is expanding. This deflection is in the x-y plane which could be an issue for the Wyko in that it measures more accurately in the z-axis.

![3D image of vernier structure.](image2.png)
Once a deflection is determined, it must be put into a model in Comsol Multiphysics which is a finite element analysis program. This must be done because even though the beam is pure SiO₂, the area surrounding it and holding the floating beam is still silicon. Thus, the solution is not simply putting a number into an equation; the thermal expansion of the silicon must also be taken into account and thus it must be modeled rather than calculated.

Figure 3 shows the other structure tested, a cantilever beam structure. Using another metal to form a bimetallic strip, the cantilevers will curl based on a temperature change. The idea with the bimetallic strip is that with mismatched coefficients, one material will expand or contract faster than another causing the combination material to curl. This curl can be measured and put into an equation and thus the coefficient can be calculated for. The larger number of cantilevers also means a greater statistical chance for good data as well as giving a good range of items to test across.

A thin gold film will be deposited onto the samples thus providing a film of gold atop the cantilever structures. The thin film gold was deposited using a table top system typically used for coating samples for a SEM. The gold film was approximately 250-300Å thick. While this is relatively thin, it is taken into account when calculating for the coefficient and should still provide the desired curl.

\[
\alpha_z = \alpha_f - \frac{[E_1 h_1^4 + 4E_2 E_1 h_1 h_2 + 6E_1 E_2 h_1^2 h_2^2 + 4E_1 E_2 h_1 h_2^3 h_3 + E_2 h_2^4]+k}{6E_1 E_2 (h_1 + h_2)h_2 h_3 \Delta T}
\]

Equation 1. Curl based coefficient calculation.

Equation 1 shows the equation used to calculate for the coefficient of thermal expansion where \( \alpha \) is the coefficient, \( k \) is the curvature of the beam, \( E \) is the Young’s modulus of the material, \( h \) is the thickness of the material and \( \Delta T \) is the change in temperature. Based on outputs from the Wyko system, the coefficient can be calculated.

Table 1. Calculated coefficients from cantilevers.

<table>
<thead>
<tr>
<th>Size (μm x μm)</th>
<th>°C⁻¹</th>
<th>Temperature Change (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20x20</td>
<td>1.32E-05</td>
<td>180</td>
</tr>
<tr>
<td>20x40</td>
<td>1.35E-05</td>
<td>180</td>
</tr>
<tr>
<td>20x60</td>
<td>1.19E-05</td>
<td>180</td>
</tr>
</tbody>
</table>

Discussion

The first item to note is that no results were retrieved with the vernier type structures. This is because no reliable measurable deflection could be determined. As stated previously, the Wyko is more sensitive in the z-axis versus the x-y plane which could have attributed to this. Similarly, the devices may be too large for a single film to react in such a way that would be measurable. Therefore, these devices need to be redesigned if they are to be used in the future for this type of work.

Table 1 shows the calculated coefficients from the cantilever structures. These were the three shortest structures all with a similar width of 20μm. Beyond the 3rd cantilever, the data became unreliable. This could be due to several factors but what was assumed was that the cantilevers were too long for the pit etched below them in that the cantilevers did not have enough room to show a change in curvature because they had already touched the bottom of the pit. One way these devices could be improved in the future would be to deepen this etch pit so that the longer cantilevers will have the maximum radius to curve.

Another item to note about the data retrieved is that it is significantly higher than published values for similar coefficients. This could be due to several things mainly dealing with the thin film gold deposited as the second material in the bimetallic stack. Assumptions were made about the thickness, modulus and other various components. As stated previously, this experiment was in part a show of methodology in that it was partially about showing that the methodology could work and coefficients could be calculated so as this is an issue for the immediate calculations, it does not affect the methodology portion of the experiment.

Extension

An additional part of the experiment that was tested was a dynamic MEMS test performed on the
cantilever structures. The resonant frequency was the item of interest in this portion of the experiment. Using the Wyko, the same environmental chamber and piezo resonator, the resonant frequency was sought after. The idea was to change the temperature of the devices and observe any change in resonant frequency.

Unfortunately, because of the size of the devices, the resonant frequency was too high to be readily measured with the available equipment. Again, the devices could be tuned for this type of measurement in the future.

Conclusions

Overall, the experiment was a success more in the sense of proving the method versus actually measuring a coefficient. In the future, the vernier structures should be made smaller to be more affected by the temperature changes and thus produce more of a measurable deflection. Similarly, some process tuning is necessary with the cantilevers with regard to the gold film.

References


[6] NSF MRI grant ref: ECCS-0619676, Karl D. Hirschman (PI). “Acquisition of an Optical Profiler for Surface Characterization and Dynamic Analysis of MEMS Devices,” Award Date: 9/01/06 Funding amount: $223,507
