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Determining thermal expansion coefficients of thin films using micromachined cantilevers

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Abstract

In this research, the coefficient of thermal expansion (CTE) of thin films was studied through analytical and experimental approaches using micromachined beams. Both single layer and bilayer micromachined cantilevers (microcantilevers) were exploited in measuring the thermal expansion of the thin films. It was obtained that both single and bilayer micromachined cantilevers would exhibit an out of plane deflection after subjected to temperature changes. Thus the thermal expansion of thin film materials can be determined using optical interferometric techniques on these heat-deformed microcantilevers. The contributions of the proposed techniques are that they can be used to increase the sensitivity and accuracy of CTE measurements. Furthermore, the distribution of the thin film CTE across the entire substrate can also be determined through the proposed approaches. Since the microcantilever structure used in this study is very simple, both modeling and fabrication processes are simplified. Thus the proposed technique can be applied to supplement other techniques used in determining the CTE of thin films.

Keywords: Thin film; Coefficient of thermal expansion; Micromachined cantilever

1. Introduction

Presently, the mechanical properties of thin films, for instance the residual stresses [1], elastic constants [2], Poisson's ratio [3], and the thermal conductivity [4], have been studied extensively. Based on the results from these researches, it is obtained that the mechanical properties of thin films may not be the same as that of the bulk materials. In addition, the mechanical properties of thin films can even depend upon the film thickness and the fabrication processes used [5]. Hence it is more reliable to directly characterize the mechanical properties from the thin film to be determined. Thermal expansion is an important mechanical behavior in MEMS. There are several problems that arise from the thermal expansion effect; for example, the mismatch of thermal expansion between the thin films and the substrate may lead to residual stresses in the thin films [1]. Therefore damage or deformation of the micromachined structures may occur. On the other hand, the thermal expansion effect can be exploited to drive the microactuator [6,7]. In order to design micromachined devices properly, it is necessary to characterize the coefficient of thermal expansion (CTE) for thin film materials.

There are several available techniques used to measure the CTE of bulk materials [8–13]. The most widely used approaches for measuring the thermal expansion of a sample are optical methods. For instance, the expansion of a specimen results in the tilt of a mirror which shifts the reflection angle of an incident light beam on the mirror. Hence, the expansion of the specimen is measured by the rotation angle of the reflected light [8,9]. As a second example, the thermal expansion of a sample can also be designed to change the gap between two objects. Thus the CTE of the sample is measured by the shift of the interference fringes between these two objects [10,11]. However a complicated mechanical assembly is required to measure the thermal expansion of the specimen through optical methods. From the microscopic standpoint, the X-ray diffraction method is used to determine the CTE of the material by measuring the expansion of the crystal lattice [12,13].

The techniques used to determine the CTE of thin films have rarely been discussed so far. The conventional optical techniques are not appropriate for the measurement of thin film CTE since the thickness of the films are too small to

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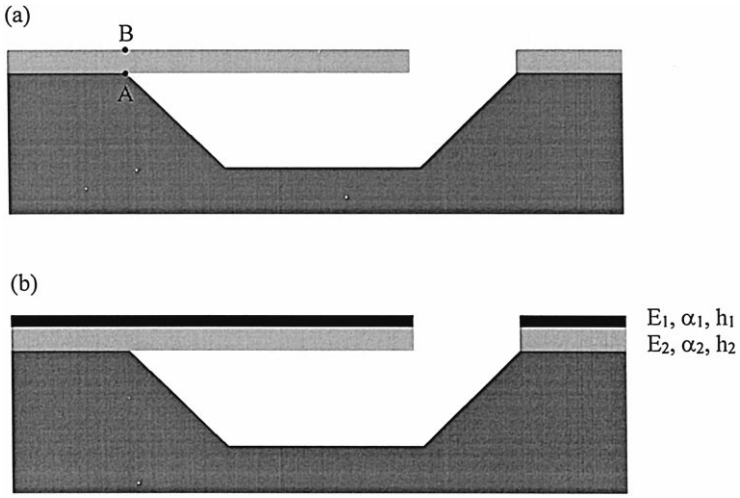

Fig. 1. (a) Single layer, and (b) bilayer microcantilever.

allow the preparation of a specimen for the experiments mentioned in [8–11]. In addition, the thin film materials cannot be used to set up the experimental apparatus for the conventional experiments. Although the X-ray diffraction method can be used to measure the CTE of thin film materials, it is only appropriate for a crystalline structure [14]. Recently, the idea of determining thin film CTE with an ellipsometer was proposed [15]. However, the variations in thickness induced by factors other than thermal expansion were not considered. In this study, the thermal expansion coefficient of thin film materials was determined using the deformation of micromachined beams through experimental and analytical approaches. The single and the bilayer micromachined cantilevers (microcantilever) illustrated in Fig. 1 were exploited in this study to measure the thermal expansion of the thin films. As a result of theoretical analysis it was obtained that both the single and bilayer microcantilevers would exhibit an out of plane deflection after subjected to temperature changes. Thus the thermal expansion of thin film materials can be determined using optical interferometric techniques upon these self-deformed microcantilevers.

2. Theoretical analysis

When the temperature is raised by ΔT, the in plane thermal expansion ΔL of a cantilever beam at its free end is

$$\Delta L = L\alpha\Delta T \tag{1}$$

where L is the initial length of the beam. Therefore the CTE of the beam can be determined from Eq. (1) if the thermal expansion ΔL is measured [16]. However, this approach is not practical for micromachined structures, since the in plane deformation ΔL of a micromachined beam under a reasonable temperature change is too small to be measured. For instance, the ΔL of a 200-μm long SiO_2 beam is only approximately 0.01 μm when the temperature is raised by 100°C. On the other hand, the out of plane deflection, such as bending in a micromachined beam, can be determined accurately by optical interferometer.

In this section, two theoretical models are established to determine the relationship of the CTE of thin films and the out-of-plane deflection of microcantilevers. In the first approach, a single layer microcantilever, shown in Fig. 1a, made from the thin film to be measured is studied. The CTE of this film was determined after the angular deflection of the microcantilever was measured. As a second approach, the thin film to be measured is deposited onto a microcantilever to form a bilayer beam as shown in Fig. 1b. The CTE of the film is then deduced using the bending of the bilayer cantilever.

2.1. Single layer microcantilever approach

As shown in Fig. 1a, the boundary of the single layer microcantilever is fixed to the substrate on only one surface. When the temperature is increased, the points A and B indicated in Fig. 1a will move as a result of the in plane expansion of the thin film and the substrate. The moving distance of points A and B will be different if the CTE between the substrate and the thin film is different.

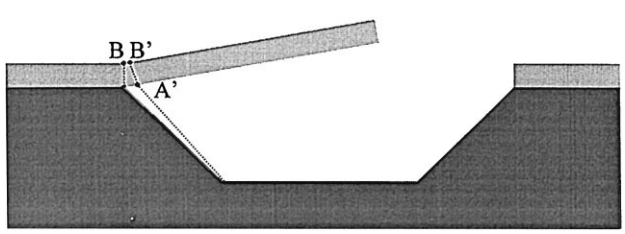

Fig. 2. The displacement at the boundary of the microcantilever at an elevated temperature.

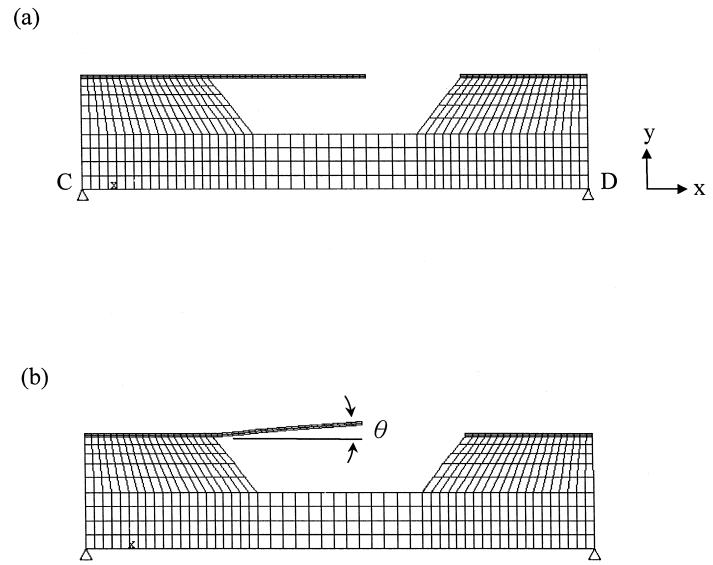

Fig. 3. (a) Finite element model for the microcantilever and the silicon substrate, and (b) the deformation of the microcantilever analyzed by the model at an elevating temperature.

Thus the microcantilever is supported by a deformed boundary A′B′ after thermal expansion, as shown in Fig. 2, and then experiences an angular deflection of θ.

As shown by the meshes in Fig. 3a, a finite element model is established to analyze the two-dimensional stress state and deformation of the single layer microcantielver. The finite element model includes the silicon substrate and a microcantilever made of the thin film to be measured. At the boundary of this model, all of the nodes except C and D, as indicated in Fig. 3a, are free to expand in both the x and y directions. On the other hand, the nodes C and D are allowed to expand in the x direction but not in the y direction. An angular deflection, θ, of the cantilever occurs after the model in Fig. 3a is subjected to a temperature change. The typical results from the model after the temperature was increased to 100°C is shown in Fig. 3b. According to the results from the finite element analysis, the relationship between angular deflection θ and the CTE α of the thin film is shown in Fig. 4. After parameter studies with the model provided, the empirical representation of θ and the other parameters is

$$\theta = \frac{3.86\times10^{-4}\Delta T\Delta\alpha(0.92+0.10t-0.02t^2)(0.95+0.35\nu)}{(2.98\times10^{-4}-1.32\times10^{-16}\Delta E)} \qquad (2)$$

where t and ν are the thickness and Poisson's ratio, respectively of the thin film, ΔT is the rising temperature, and ΔE and $\Delta\alpha$ are the difference in values for the elastic constant and CTE, respectively between the substrate and the film. In the finite element model, the elastic constant and the CTE of the silicon substrate are 190 GPa and 2.6×10^{-6}/°C, respectively [17]. In addition, the Poisson's ratio of the silicon substrate is assumed to be 0.15. Eq. (2) has been evaluated over 0.2 μm $\le t \le$ 2 μm, 50 GPa $\le \Delta E \le$ 180 GPa, and -30×10^{-6}/°C $\le \Delta\alpha \le 30\times10^{-6}$/°C and appears to well represent θ within this parameter range. The substrate modeled in Fig. 3 is only 40 μm thick in order to reduce the computational time. In fact, the difference between the results from a finite element model with a 40 μm thick substrate and one with a 500 μm thick substrate is less than 1%. Further, the deviation of the result is only 1.4% if the Poisson's ratio of the silicon substrate is increased from 0.15 to 0.3.

2.2. Bilayer microcantilever approach

As schematically shown in Fig. 1b, a bilayer cantilever consists of two different thin film materials. The bilayer

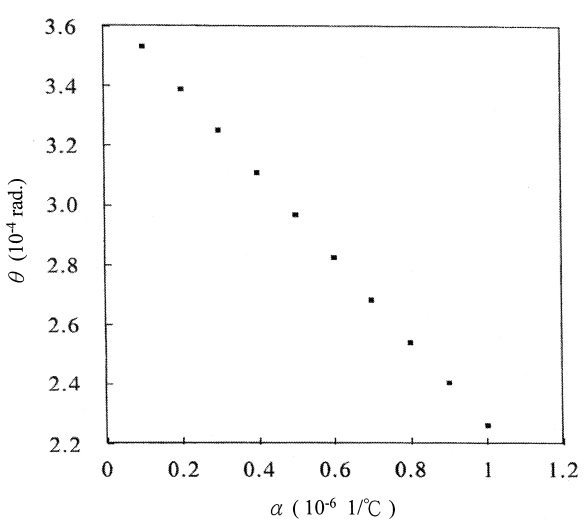

Fig. 4. Relationship between the CTE of the thin film and the angular deflection of the microcantilever.

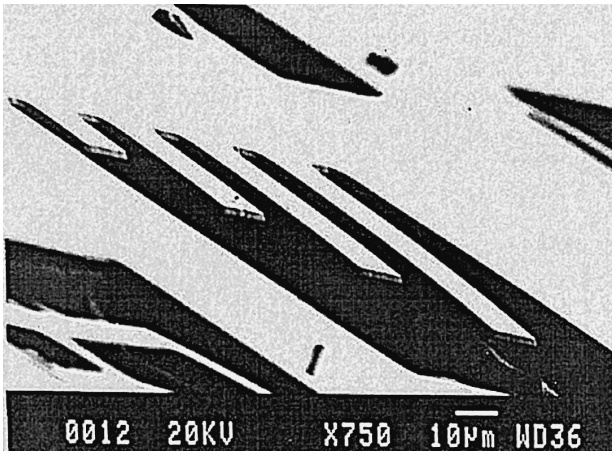

Fig. 5. The SEM photo of four bilayer microcantilevers.

cantilever will be bent with a radius of curvature ρ after experiencing a temperature change if the thermal strains of these two films are different [18]. In this case, the thermal strains are introduced by the temperature change ΔT and the difference in CTE between the thin films $\Delta\alpha_f(=\alpha_1-\alpha_2)$. Through standard stress analyses, the relationship between the curvature $1/\rho$ of the bilayer beam and the difference in CTE $\Delta\alpha_f$ between the films becomes

$$\frac{1}{\rho}=\frac{6\cdot\Delta T\cdot\Delta\alpha_f\cdot(1+m)^2}{h\cdot\left[3\cdot(1+m)^2+(1+m\cdot n)\left(m^2+\frac{1}{m\cdot n}\right)\right]} \quad (3)$$

where $h=h_1+h_2$ is the total thickness of the bilayer structure, and $n=E_1/E_2$ and $m=h_1/h_2$ are two nondimensional parameters representing the ratio of values for the elastic constant and thickness, respectively between the two films.

Eq. (3) reveals that the curvature of the bilayer cantilever is a function of the difference in CTE between the two films. With m and n in Eq. (3) being determined from the measured elastic constants and thickness, the $\Delta\alpha_f$ between the thin films is found when the deflection profile of the microcantilever is measured. Hence, the CTE α_1 is determined from the $\Delta\alpha_f$ if α_2 has been found.

3. Experiment and results

The CTE of SiO_2 and Al films have been used in applications of this technique in case studies. The SiO_2 film was thermally grown using wet oxide at 1050°C in the experiment. The single layer SiO_2 microcantilevers with length between 40 and 200 μm were fabricated using conventional bulk micromachining. In addition, the SiO_2 film, which still bonded to the silicon substrate, is 1.13 μm thick after bulk etching. The bottom of the SiO_2 microcantilever will also be etched during bulk etching after the silicon substrate underneath is removed. Therefore, the thicknesses of the microcantilevers are ranging from 1.07 to 1.13 μm. These SiO_2 cantilevers became bilayer structures if an additional thin film was deposited onto them. In the experiments discussed, a 0.5 μm thick aluminum film was deposited using thermal evaporation. The SEM photograph shown in Fig. 5 is four bilayer microcantilevers fabricated using the above processes. In this study, the CTE of the SiO_2 film was first determined using the single layer microcantilever approach. Consequently, the CTE of the aluminum film that formed a bilayer microcantilever with SiO_2 film was determined through the bilayer microcantilever approach.

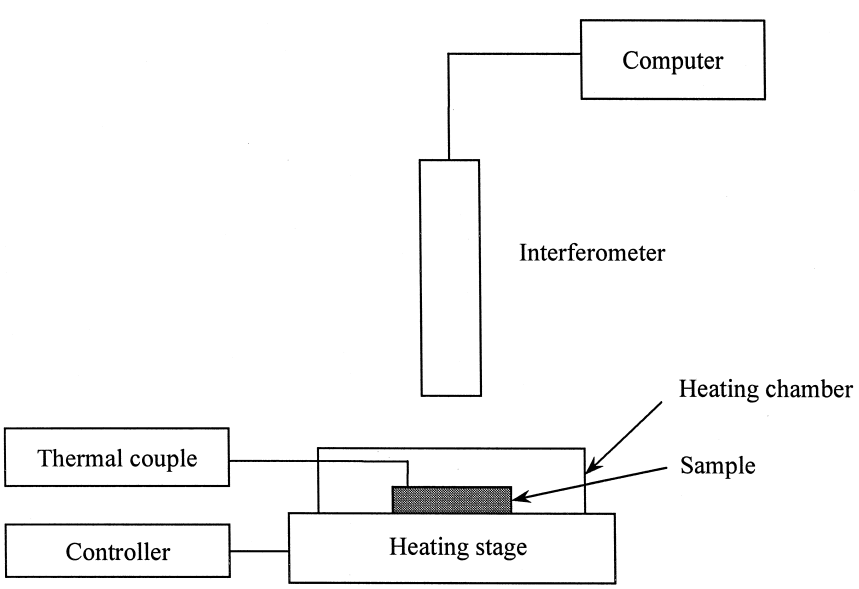

Fig. 6. A schematic of the experimental apparatus.

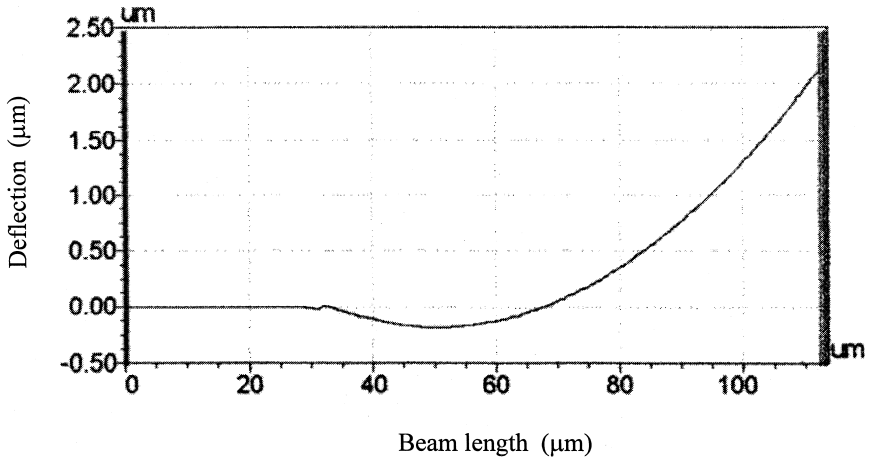

Fig. 7. A typical measured deformation profile obtained from interferometric microscope.

The sample, which contains microcantilevers, is characterized by the experimental setup shown in Fig. 6. The sample was heated by a heating stage which had a controller to maintain deviations in the temperature within 0.1°C. In order to attain thermal equilibrium, the sample was kept inside a chamber at a constant temperature for about 5 min before the measurement. As shown in Fig. 6, the temperature at the surface of the silicon substrate was monitored using a thermal couple. After the sample was heated by the heating stage, the microcantilevers was deflected out-of-plane as discussed in Section 2. The deflection profile of the microcantilever was measured using an optical interferometer. A typical deflection profile of a SiO_2 microcantilever measured through this approach is shown in Fig. 7. The flat region extended from 0 to 31 μm of the horizontal axis represents the area where the SiO_2 film is still bonded to the substrate. Consequently, the microcantilever is extended from 31 to 125 μm of the horizontal axis. According to the gradient residual stress, the microcantilever shown in Fig. 7 is bent. In addition, the microcantilever has a negative deflection induced by the boundary rotation effect [1]. After taking the data points along the length of the measured configuration of the microcantilever, the transverse deflection of the microcantilever as denoted by the symbols (dot and cross) shown in Fig. 8 was obtained. The measurements were taken on microcantilevers with different lengths and at different positions on the same wafer. Therefore, the errors associated with the deviation of any single measurement were minimized.

The CTE of SiO_2 film was determined using the single layer approach first. The data points shown in Fig. 8 were obtained from the measured profiles of the single layer SiO_2 cantilever at 30°C and 100°C. As indicated in Fig. 8, the single layer microcantilever was already deformed at room temperature. This was due to the existence of thin film residual stresses [1]. The angular deflections θ of

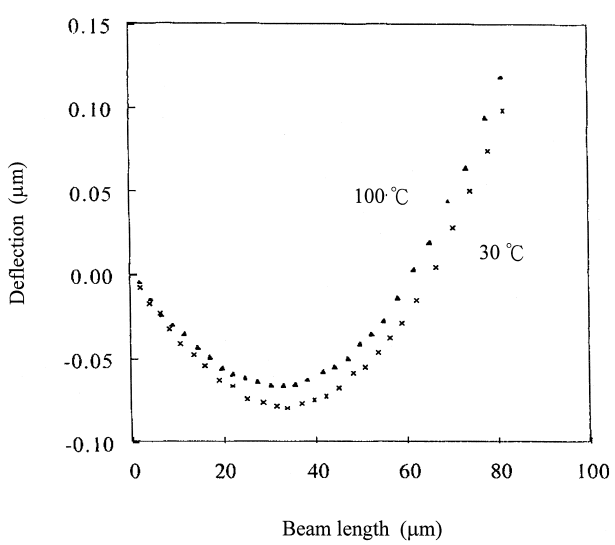

Fig. 8. The data points obtained from the measured deflection profile of single layer microcantilever at different temperature.

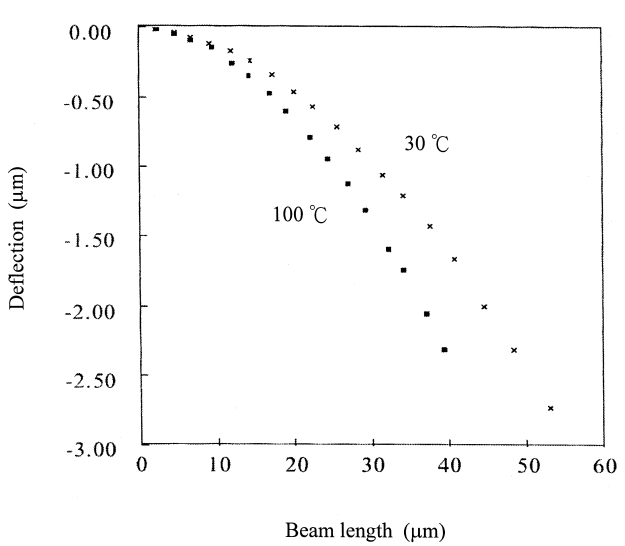

Fig. 9. The data points obtained from the measured deflection profile of bilayer microcantilever at different temperature.

these two profiles were then obtained using the curve fit. Since the CTE of SiO_2 film is smaller than the Si substrate, the angular deflection θ of the SiO_2 cantilever was counter clockwise after heating. According to the measurement, the variation of θ for the microcantilever after heated from 30 to 100°C was 3.43×10^{-4} rad. With the difference of θ, the CTE of the SiO_2 film was calculated from Eq. (2) as $0.25 \times 10^{-6}/°C$ within the temperature range of 30–100°C. In comparison with the existing results, the CTE of bulk SiO_2 $0.4 \times 10^{-6}/°C$ [19] and $0.55 \times 10^{-6}/°C$ [20] were also reported.

As a second example, the CTE of a thermal evaporated Al film was determined using the bilayer (SiO_2 and Al) microcantilever approach. The data points shown in Fig. 9 were obtained from the measured profiles of the bilayer cantilever at 30°C and 90°C. Due to the existence of thin film residual stresses [1], the bilayer microcantilever was deformed at room temperature. Since the CTE of Al film is greater than that for SiO_2 film, the curvature of the bilayer cantilever is increased after heating. Hence the variation in the radius of curvature for the bilayer microcantilever after heating from 30 to 90°C is 400 μm (i.e., from 1150 to 750 μm). With a difference of the $1/\rho$, the $\Delta\alpha_f$ between SiO_2 and Al film was calculated from Eq. (3) as $20.55 \times 10^{-6}/°C$. Since the CTE of SiO_2 film was determined through the single layer microcantilever approach to be $0.25 \times 10^{-6}/°C$, the CTE of Al film is $20.30 \times 10^{-6}/°C$ within the temperature range of 30–90°C. In comparison with the existing results, the CTE of bulk Al is $23 \times 10^{-6}/°C$ [17] and $25 \times 10^{-6}/°C$ [20].

4. Discussion

In this research, the CTE of thin films was studied through analytical and experimental approaches using microcatilevers. The fabrication processes required for the single layer microcantilever technique is more straightforward. On the other hand, the bilayer microcantilever technique is especially useful for making measurements on very thin films since microcantilevers are not readily fabricated of such thin materials. The contribution of the proposed techniques is that they can be used to increase the sensitivity and accuracy of CTE measurements. Further, the distribution of the thin film CTE across an entire substrate can also be determined through the proposed approaches. Since the microcantilever structure used in this study is very simple, both modeling and fabrication processes are simplified. Thus the proposed technique can be applied to supplement other techniques in determining the CTE of thin films.

In this experiment, the change of the curvature for bilayer microcantilever becomes insignificant for some of the thin film materials. Therefore, the errors for measured CTE can be remarkable. For instance, the CTE of sputtered Tungsten (W) thin film measured through a bilayer cantilever consisting of sputtered W and thermal SiO_2 was distributed from $4.5 \times 10^{-6}/°C$ to $6.9 \times 10^{-6}/°C$. In other word, the deviation of the measured results can even reach 50% high. In comparison with the existing results, the CTE of bulk W is $4.5 \times 10^{-6}/°C$ [17,20]. This is mainly because the difference in CTE and the ratio of elastic constants between W and thermal SiO_2 films are large. In this experiment, the ratio of elastic constant is approximately $n = 1$ for Al film, but is $n = 6$ for W film. The difference of CTE is estimated to be $\Delta\alpha = 20 \times 10^{-6}/°C$ for Al film, but is only $\Delta\alpha = 4 \times 10^{-6}/°C$ for W film. According to Eq. (3), the change of $1/\rho$ is not significant for small $\Delta\alpha$ and large n. This condition limits the materials that can be measured using the proposed technique.

Due to the existence of the creep effect, the deformation of a structure may occur gradually with time after subjection to a load. The composition of thin films could be changed at higher temperatures due to the motions of atoms, vacancies, dislocations, etc. within a solid material occur more rapidly [21]. Hence, the creep effect becomes significantly at higher temperature. The thin film is often subjected to the residual stresses generated by the fabrication processes. In other words, the deformation of the microcantilever may vary with time during the experiment due to the occurrance of the creep effect by residual stress and thermal loading. For example, the deformation profile of a bilayer cantilever constituted by thermal SiO_2 and evaporated Al is shown in Fig. 10a. The deflection profile of the cantilever is changed in Fig. 10b after the sample is

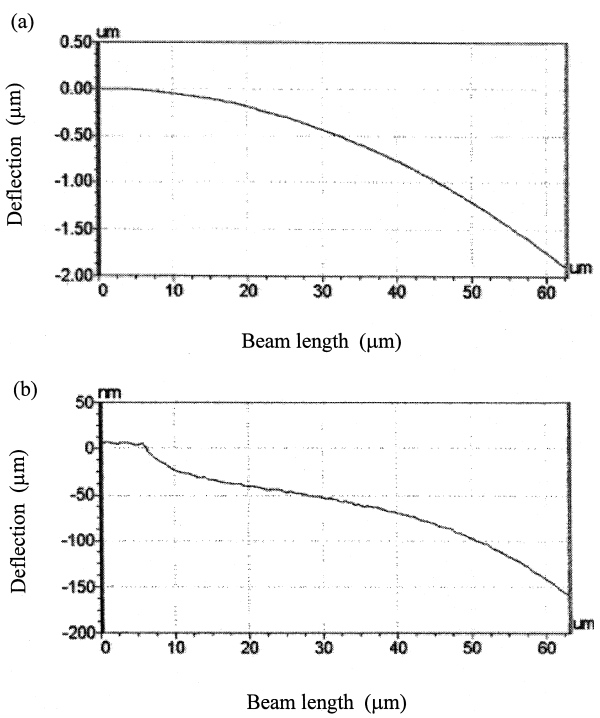

Fig. 10. The variation of the deflection profile for bilayer microcantilever at different time.

heated at 100°C for 3 h. It is believed that this behavior is due to the creep of the Al film by residual stresses and thermal loading during heating. Consequently, the heating time in this experiment cannot be too long for some of the thin films. Thus the measurements for this experiment were conducted immediately after the sample reached the designated temperature to prevent the creep effect.

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