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Sensors and Actuators 84 (2000) 310–314

SENSORS AND ACTUATORS A PHYSICAL

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On the thermal expansion coefficients of thin films

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Received 9 July 1999; received in revised form 15 November 1999; accepted 21 December 1999

Abstract

The coefficient of thermal expansion (CTE) is an important mechanical property for thin film materials. There are several problems that arise from the thermal expansion effect; for example, the mismatch of thermal expansion between the thin films and the underlying substrate may lead to residual stresses in the thin films. On the other hand, the thermal expansion effect can be exploited to drive microactuators. The CTEs of Al and Ti thin films were determined in the present study using the bilayer microcatilever technique. The contribution of this paper is to demonstrate the variation of the thin film CTE with the film thickness. The CTE of the Al thin film changes from $18.23 \times 10^{-6}/°C$ to $29.97 \times 10^{-6}/°C$, when the film thickness increases from 0.3 to 1.7 μm. The CTE of the Ti thin film changes from $21.21 \times 10^{-6}/°C$ to $9.04 \times 10^{-6}/°C$, when the film thickness increases from 0.1 to 0.3 μm. Further, the concept that thin film CTE may be influenced by the defects in thin film materials is proposed. Thus, a desired thin film CTE can be obtained by tuning the film thickness as well as the deposition conditions.

Keywords: Thermal expansion coefficients; Thin film

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1. Introduction

Thermal expansion is an important mechanical behavior in the areas of microelectronics and microelectromechanical systems (MEMS). There are several problems that arose from the thermal expansion effect, for instance, the mismatch of thermal expansion between the thin films and the substrate may lead to residual stresses in the thin films [1]. Thus, the electronic devices as well as the micromachined structures will be damaged or deformed by this effect. On the other hand, the thermal expansion effect can be exploited to drive microactuators [2,3]. In order to design micromachined components as well as microelectronics 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 [4–7]. However, the thickness of the films are too small to be determined using the conventional optical techniques [4–7]. Although the X-ray diffraction method can be used to measure the CTE of thin film materials, it is only appropriate for crystalline structures [8–10]. The idea of determining thin film CTE with an ellipsometer was available [11]. However, the variations in thickness induced by factors other than thermal expansion were not considered. In Ref. [12], the thermal expansion coefficient of thin film materials was determined using the deformation of micromachined cantilever (microcantilever). Thus, the thermal expansion of the film with a very small thickness can be determined accurately in this manner.

It is obtained that the mechanical properties of thin films, such as the residual stresses [1] and the elastic constants [13], may not be the same as those of the bulk materials. The mechanical properties of thin films can even depend upon the film thickness and the fabrication processes used [14]. Hence, it is more reliable to directly characterize the mechanical properties from the thin film to be determined. In this study, the approach presented in Ref. [12] is exploited to determine the CTEs of the aluminum and titanium films. The variation of the CTEs of Al and Ti films with their film thickness is also discussed. According to the experimental results, the difference of the CTE between the bulk and thin film materials is signifi-

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PII: S0924-4247(00)00311-3

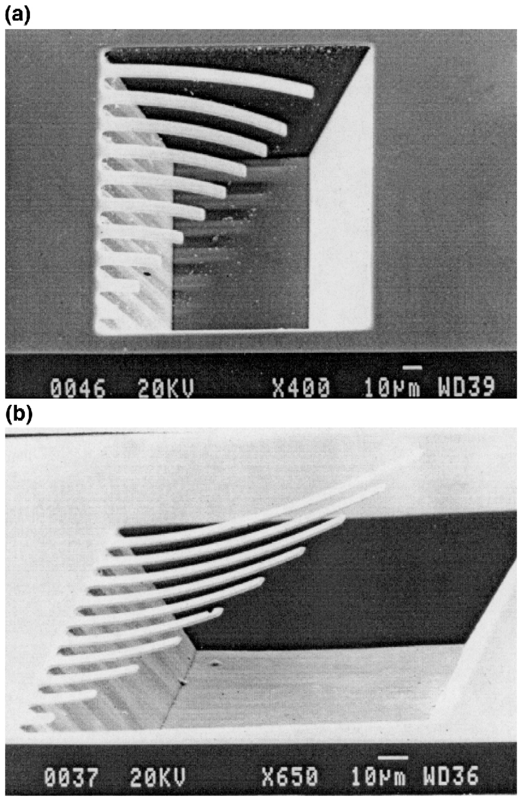

Fig. 1. The SEM photographs of the bilayer microcantilevers consist of (a) SiO_2 and Al, and (b) SiO_2 and Ti.

cant. In addition, the CTE of thin films vary remarkably with the film thickness.

2. Experiment and results

In this study, the thermal SiO_2 film was used to fabricate microcantilever arrays. After a 1.1-μm thick SiO_2 film was thermally grown using wet oxidation at 1050°C, the SiO_2 microcantilever array with cantilever between 40 and 200 μm long were fabricated using bulk micromachining. The bilayer microcantilevers were obtained after an additional Al as well as Ti film was deposited onto the SiO_2 cantilevers. Thus, the CTE of Al and Ti films were measured using the bilayer technique presented in Ref. [12]. In the experiments discussed, the aluminum films with thickness ranging from 0.3 to 1.7 μm were deposited using thermal evaporation. In addition, the titanium films with thickness ranging from 0.1 to 0.3 μm were deposited using electron beam evaporation. The SEM photographs shown in Fig. 1 are the bilayer microcantilever array fabricated using the above processes.

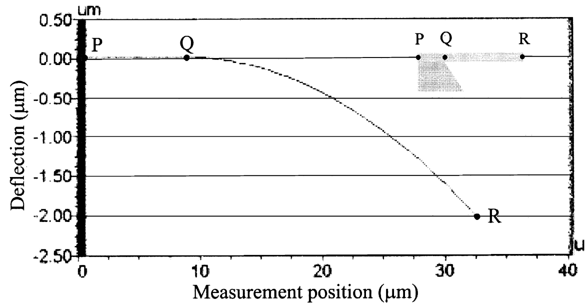

Fig. 3. A typical measured deformation profile of Al film obtained from interferometric microscope.

The test sample, which contains bilayer microcantilevers, is characterized by the experimental setup shown in Fig. 2 [12]. The test 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. 2, the temperature at the surface of the silicon substrate was monitored using a thermal couple. Since the bilayer microcantilever consisted of two thin films with different CTEs, it was bent out of plane after the sample heated by the heating stage. The deflection profile of the microcantilever was measured using the

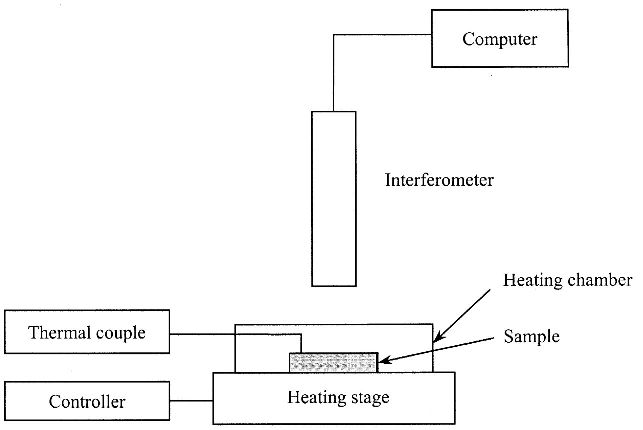

Fig. 2. A schematic of the experimental apparatus.

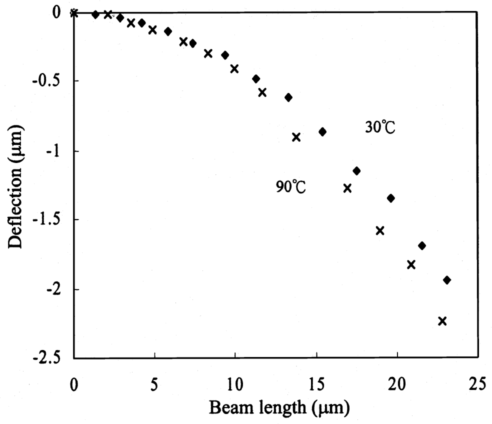

Fig. 4. The data points obtained form the measured deflection profile of a Al/SiO$_2$ bilayer microcantilever at different temperatures.

optical interferometer shown in Fig. 2. According to the change of the radius of curvature of the bilayer microcantilever, the CTE of the Al and Ti films were determined.

2.1. Aluminum thin film

The typical out-of-plane deflection configuration of a Al/SiO$_2$ bilayer microcantilever measured by the optical interferometer is shown in Fig. 3. The bilayer microcantilever consisted of a 1.0-μm thick Al and 1.1-μm thick SiO$_2$. The profile shown in Fig. 3 is measured along the path P → Q → R indicated in the inset. Thus, the region at the left-hand side of point Q represents the thin film that still bonded to the substrate. On the other hand, the region at the right hand side of point Q represents the deformation configuration of the microcantilever that suspended above a cavity. According to the measurement, the bilayer microcantilever had already been bent at room temperature. This was mainly due to the existence of residual stresses for Al thin film [1]. It is also obtained from Fig. 3 that the Al thin film is under residual compression since the bilayer microcantilever is bent downward [14].

The data points shown in Fig. 4 were obtained from the measured profiles of the bilayer cantilever at 30°C and 90°C. The curvature of the bilayer cantilever increases after heating since the CTE of Al film is greater than that of SiO$_2$ film. Hence, the variation in the radius of curvature ρ for the bilayer microcantilever after heating from 30°C to 90°C is -35 μm (i.e., from 277 to 242 μm). With a change of the $1/\rho$, the difference of CTE $\Delta\alpha$ between SiO$_2$ and Al film was calculated as 23.20×10^{-6}/°C. Since the CTE of SiO$_2$ film was determined through the single layer microcantilever approach to be 0.25×10^{-6}/°C [12], the CTE of the 1.0-μm thick Al film is 23.45×10^{-6}/°C within the temperature range of 30°C to 90°C. The CTEs of the Al films for five different thicknesses were determined in the same manner as well. As shown in Fig. 5, the CTE of the Al thin film varies from 18.23×10^{-6}/°C to 29.97×10^{-6}/°C, when the film thickness increases from 0.3 to 1.7 μm. The measurement had been conducted for microcantilevers located at five different arrays on the same wafer. The data points in Fig. 5 denote the average measured value, and the vertical bars indicate the highs and lows that were recorded over the ensemble of measurements. In comparison with the existing results, the CTE of bulk Al is 23×10^{-6}/°C [15].

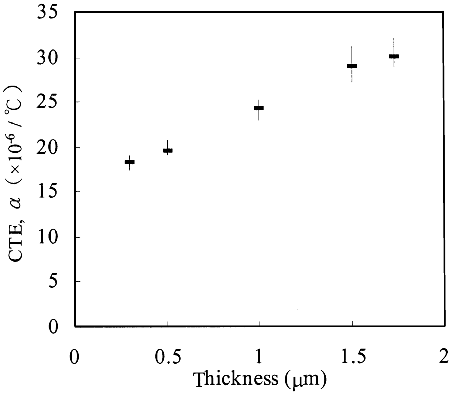

Fig. 5. Variation of the CTE and film thickness for Al film.

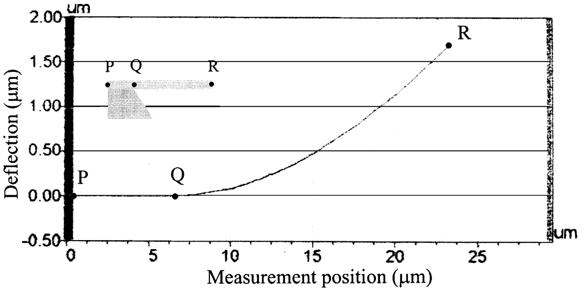

Fig. 6. A typical measured deformation profile of Ti film obtained from interferometric microscope.

2.2. Titanium thin film

The typical out-of-plane deflection configuration of a Ti/SiO$_2$ bilayer microcantilever measured by the optical

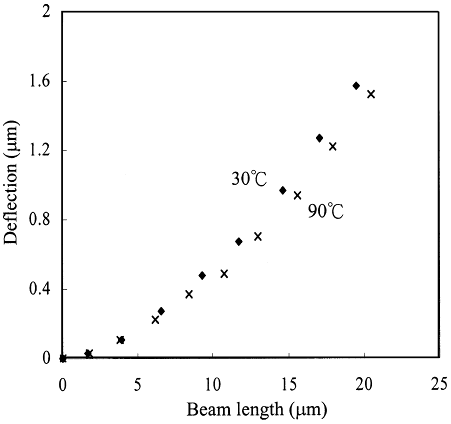

Fig. 7. The data points obtained form the measured deflection profile of a Ti/SiO$_2$ bilayer microcantilever at different temperatures.

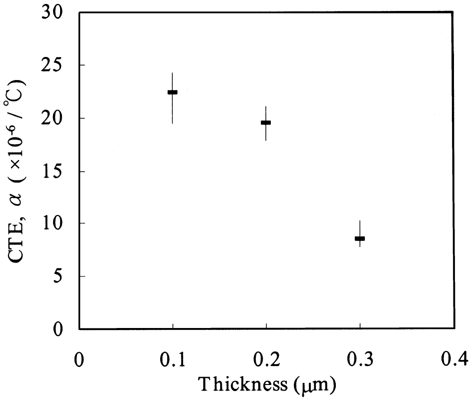

Fig. 8. Variation of the CTE and film thickness for Ti film.

interferometer is shown in Fig. 6. The bilayer microcantilever consisted of a 0.2-μm thick Ti and 1.1-μm thick SiO_2. The profile shown in Fig. 6 is also measured along the path $P \rightarrow Q \rightarrow R$ indicated in the inset. Due to the existence of residual stresses for Ti thin film, the bilayer microcantilever was also bent at room temperature. It is obtained from Fig. 6 that the Ti thin film is under residual tension since the bilayer microcantilever is curved upward [14].

The data points shown in Fig. 7 were obtained from the measured profiles of the bilayer cantilever at 30°C and 90°C. Since the CTE of Ti film is greater than that for SiO_2 film, the curvature of the bilayer cantilever decreases after heating. Thus, the difference of the radius of curvature ρ for the bilayer microcantilever is 55 μm (i.e., from 303 to 358 μm) after heating from 30°C to 90°C. With a change of the $1/\rho$, the difference of CTE $\Delta\alpha$ between SiO_2 and Ti film was calculated as 19.84×10^{-6}/°C. Thus, the CTE of the 0.2-μm thick Ti film is 20.10×10^{-6}/°C within the temperature range of 30°C to 90°C. In the same manner, the CTEs of the Ti films for three different thicknesses were determined. As shown in Fig. 8, the CTE of the Ti thin film changes from 21.21×10^{-6}/°C to 9.04×10^{-6}/°C, when the film thickness increases from 0.1 to 0.3 μm. The data points in Fig. 8 also denote the average value for the measurement on five different arrays, and the vertical bars indicate the highs and lows that were recorded over the ensemble of measurements. In comparison with the existing results, the CTE of bulk Ti is 9.5×10^{-6}/°C [15].

3. Discussion

It is obtained from the experiment that the CTE of the Al film differs by 66% when the film thickness increases from 0.3 to 1.7 μm. On the other hand, the CTE of the Ti film differs by 60% when the film thickness increases from 0.1 to 0.3 μm. Consequently, the CTEs of thin film materials are very sensitive to the variation of film thickness. The experimental results also show that the CTE of the Al film is close to that of the bulk Al when the film thickness is nearly 1 μm. However, the difference of the CTEs between the bulk and the thin film Al increase with the film thickness when it is greater than 1 μm. In other words, the CTE of the thin film does not converge to that of the bulk material when the film thickness increases. In short, the CTE of thin film materials are not only affected by the film thickness.

According to the fabrication processes, residual stresses are normally generated into thin film materials [16]. In order to investigate the variation of the thin film CTEs at various film thickness, the residual stresses of the thin film materials were characterized. The residual stresses of the thin films were determined using the approach presented in Ref. [1]. The measurement had been conducted for microcantilevers located at five different arrays on the same wafer. The data points in Fig. 9 denote the average measured value, and the vertical bars indicate the highs and lows that were recorded over the ensemble of measurements. Fig. 9a shows the measured residual stresses for the Al thin films with thickness ranging from 0.3 to 1.7 μm. It is obtained that the Al film with its thickness within the measurement range is under compression. The Al film is evidently placed into higher residual compression for a substantially thicker film as indicated in Fig. 9a. Fig. 9b shows the measured residual stresses for the Ti thin film with thickness ranging from 0.1 to 0.3 μm. As opposed to

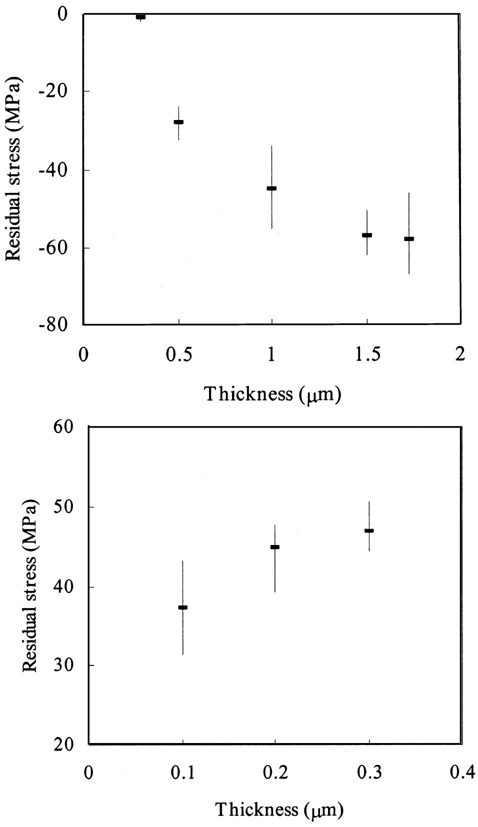

Fig. 9. Variation of the residual stress and film thickness for (a) Al film, and (b) Ti film.

the Al film, the Ti film with its thickness within the measurement range is under tension. In addition, the thicker Ti film has higher residual tension.

The residual stress of thin films deposited through the low temperature processes, such as sputtering and evaporation, is due to the accumulation of crystallographic flaws [16]. For instance, the residual compression of the Al film is due to defects of the thin film led by the trapped impurities. Thus, the number of atoms per unit length, N_a, for a Al film increases with the film thickness due to the increasing of trapped impurities. On the contrary, the residual tension of the Ti film is caused by the trapped vacancies and gaps of thin film. The N_a for Ti film decreases with the film thickness due to the increasing of trapped vacancies and gaps. The thermal expansion of a material is generated by the increase of the average interatomic distance during heating [10]. The thicker Al film has a larger thermal expansion, since the N_a increases with the Al film thickness, whereas the thicker Ti film has a smaller thermal expansion since the N_a decreases with the Ti film thickness. This result agrees with the phenomena obtained in Fig. 5 and Fig. 8. Consequently, defects in thin film serve as one of the primary mechanisms to change the CTEs of thin film materials.

4. Conclusion

The CTEs of Al and Ti thin films were determined in the present study using the bilayer microcantilever technique. In addition, the CTEs of Al and Ti thin films for various film thicknesses were also characterized. The contribution of this paper is to demonstrate the variation of the thin film CTE with the film thickness. Further, the concept that thin film CTE may be significantly influenced by the defects of the thin film materials is proposed. Thus, a desired thin film CTE can be obtained by tuning the film thickness as well as the deposition processes.

Acknowledgements

This material is based (in part) upon work supported by the National Science Council (Taiwan) under Grant NSC 88-2212-E007-004. The author would like to express his appreciation to the Electrical Engineering Department of National Tsing Hua University (Taiwan), Semiconductor Center of National Chiao Tung University (Taiwan), and National Nano Device Laboratories (Taiwan) for providing fabrication facilities.

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Biographies

Weileun Fang was born in Taipei, Taiwan, in 1962. He received his PhD degree from Carnegie Mellon University in 1995. His doctoral research focused on the determination of the mechanical properties of thin films using micromachined structures. In 1995, he worked as a postdoctoral research at Synchrotron Radiation Research Center, Taiwan. He is currently an associate professor at Power Mechanical Engineering Department, National Tsing Hua University, Taiwan. His research interests include MEMS with emphasis on microactuators and the characterization of the mechanical properties of thin films.

Chun-Yen Lo was born in Taichung, Taiwan, in 1974. He received his MS degree from National Tsing Hua University in 1999. His research is focused on the thermalmechanics of the thin films.