

Numerical Simulation of Thermal Stress in Sputtered TiB₂ Films by Finite Element Method

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Abstract—The thermal stress was generated in sputtered TiB₂ films during the films cooled down due to the mismatch of thermal expansion coefficient. As a considerable distinction in the physical and thermal properties of films-substrate system was existed, the thermal stress was still important despite of sputtering at lower temperature. The coupled field quadratic element PLANE13 was used to fabricate the combinational system model, and the finite element analysis codes (ANSYS) was employed to analyze the influence of deposition temperature and cooling velocity on thermal stress. From the results, it is found that the thermal stress increases with the rising of two technical parameters. However, the simulation exhibits a larger magnitude of the thermal stress distributed on the center in comparison to that on the edge of films-substrate system. Moreover, the thermal stress reduction at the interface was found.

Keywords-TiB₂ films; Simulation; Temperature; Thermal stress

I. INTRODUCTION

Titanium diboride (TiB₂) has been widely used as a heat-resistant ceramic owing to its unique properties, e.g. higher hardness, excellent thermal conductivity, wear resistance, and chemical stability, etc.^[1]. Recently, TiB₂ has been conventionally applied in the potential coatings or films material for various applications to the diffusion barriers in microelectronic devices^[2, 3], thermal oxidation and wear reduction coatings for cutting tools^[4], and corrosion protection especially^[5]. TiB₂ films have been deposited by physical vapor deposition (PVD) techniques, such as reactive sputtering^[6], arc evaporation^[7], and magnetron sputtering^[8]. Among such deposition methods employed, magnetron sputtering is attractive owing to its high deposition rate, low deposition temperature and possibility of using substrates with complicated geometries^[9]. However, it is still hard to prepare the TiB₂ films with good mechanical integrities because of the high residual stress in sputtered TiB₂ films, which deteriorated the mechanical integrity of the films-substrate system^[10, 9]. The high residual stress existed in films can directly influence

their properties, such like adhesion, fatigue strengthen, bond strength, tribological properties, etc.^[11-13]. Moreover, excessive residual stresses in films may cause defect formation and delamination at the films-substrate interface.

Residual stress in the sputtered films is a stress without external loading, which results from the growth stress and thermal stress. The growth stress was accepted as the main component of residual stress in sputtered films, and was investigated widely^[14]. Thermal stress result from the mismatch of the thermal expansion between the coating and the substrate and large temperature deviations when the films cooling down to room temperature after deposition. Usually, thermal stress in the films is relatively small and can be neglected approximately; however, it would be crucial when the films deposited at high temperature or with large mismatch of the thermal expansion coefficient between films and substrate. For example, it has been proved that the annealing temperature substantially affects the electrical properties of TiB₂ films^[15]. This is because the deposition temperature of TiB₂ films is above 300 °C^[9, 13], and the thermal stress proportion to a total stress is more significant^[6]. Thus, it is necessary to understand and control the thermal stress in TiB₂ films.

Although thermal stress can be measured by the experimental device equipped with a temperature chamber^[16], it needs to obtain from temperature distribution analyses previously. As a result, analytical methods become the essential way to acquire thermal stress. In the early studies, thermal stress can be obtained by the analytical equations, which was used to describe the biaxial thermal stress in films-substrate system^[17]. Currently, the numerical methods such as finite element analysis (FEA) have been regarded as an interested tool to simulate thermal stress in combinational system^[18, 19]. However, less research on the thermal stress in sputtered TiB₂ films has been reported to date^[20]. The present paper aims at the effect of deposition temperature and cooling

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velocity on the distribution of thermal stress developed in thin TiB₂ films sputtered on 316L stainless steel substrate.

II. NUMERICAL SIMULATION PROCEDURES

A. Model Definition.

For analyzing the residual thermal stress generated in sputtered TiB₂ films, especially for the distribution of thermal stress between films and substrate, a simple 2D planer model shaped 316L stainless steel sample (50μm thick) with the films (1μm thick) was fabricated. It can be seen that the substrate thickness was larger in comparison to the films thickness. The dimensions would be allowed films-substrate system to bend upon the developed of thermal stress produced in films. A schematic illustration about the physical and thermal properties of TiB₂ films and 316L stainless steel substrate are given in Table1. To simplify the thermal stress analysis, several assumptions were made as following:

TABLE 1 PHYSICAL AND THERMAL PROPERTIES OF FILMS SUBSTRATE

Properties	Materials	
	TiB ₂ films	316L stainless steel
Yong's modulus (GPa)	600	195
Poisson's ratio	0.12	0.3
Density (Kg·m ⁻³)	4520	7980
Thermal expansion coefficient (10 ⁻⁶ m·K)	8.1	18

(1) In consideration of the quite thin model, the biaxial thermal stress was regarded along with the uniform temperature maintained over the model at the deposition temperature as well as after cooling down.

(2) The films and substrate materials behaviors were isotropic and linear thermoelastic.

(3) The interface between films and substrate had a perfect bonding.

B. Simulation Details.

The simulated of thermal stress presented in sputtered TiB₂ films was performed by ANSYS finite element analysis codes. The films-substrate system was modeled using coupled field quadratic element PLANE13, and was meshed with quadrilateral-shaped elements. Based on the literature, model was meshed with the smaller size, and the higher precision was obtained at the great expense of calculating time. As stress at the films-substrate interface appears to be very complicated usually, the minimized element size across the plane was introduced near the area. All the edges of model were free so that bending was permitted to take place during cooling down.

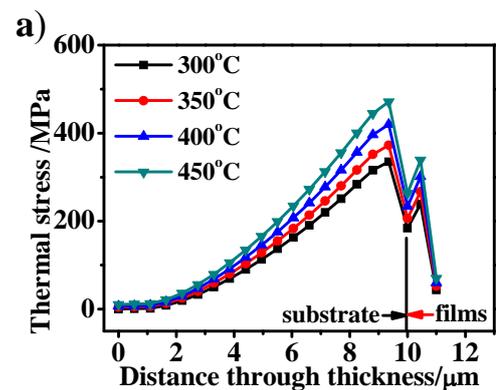
Analyses were simulated to discuss the influence of deposition temperature and cooling velocity on thermal stress by varying the values. The variety of cooling velocity can be carried out by changing the heat transfer coefficient of atmospheres in sputtered chamber. The cooling velocity ranging from 0.5 to 3.5 W/(m²·°C) with the interval of 1

W/(m²·°C) was used for simulation to evaluate the effect of cooling velocity on thermal stress, keeping the deposition temperature fixed at 350 °C. In order to understand how the deposition temperature affects thermal stress, the values of deposition temperature applied over films-substrate system vary in the range of 300 ~ 450 °C by holding the cooling velocity and room temperature as a constant value of 1.5 W/(m²·°C) and 25 °C, respectively.

III. RESULTS AND DISCUSSION

A. Deposition Temperature Studies.

Thermal stress, through the thickness of films-substrate system applied with various deposition temperatures was plotted in Fig.1. Since the deposition temperature increases ceaselessly, the generated strain derived from the mismatch of thermal expansion coefficient between films and substrate can lead to the rising of thermal stress. This phenomenon was also observed in sputtered TiN films [21]. Stress presented at the interface of films-substrate system is at a relatively lower stress level. It reveals that the stress gradient occurs at the interface. Through the thickness of combinatorial system, the stress on the center is higher than that on the edge, and the maximum is distributed in the films and substrate respectively. This is clearly seen in Fig.2. From Fig.1 (b), it shows that the stress on the center of films increases obviously. These can be explained that the strain induced by the variation of deposition temperature on the center is easy to be achieved. Meanwhile, the considerable bending-induced stress is relaxed and consequently lower stress on the edge [19]. Through the thickness of films, it is noticeable that the stress tends to increase, and then drops slowly by reason of the restraining of substrate at the bottom of films. The films failure mechanisms are generally determined by the distribution and magnitude of the stress. With the combinational system subjected to high temperature, the generation of large strain, causing great bending deformation, the stress increased dramatically following with the increasing temperature. In the case of 450 °C, the stress increases immediately and reaches a maximum. Therefore, the films sputtered at 450 °C are very prone to high stress concentration and failure.



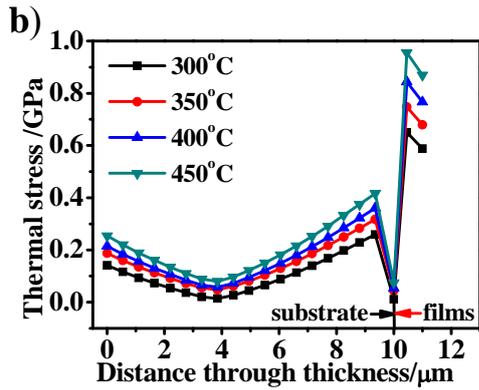


Fig.1 Thermal stress distribution through the thickness of films-substrate system with various deposition temperatures on the (a) edge; (b) center.

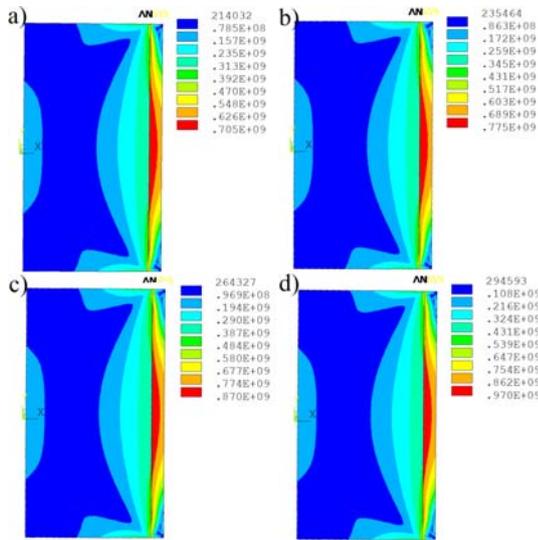


Fig.2 Thermal stress fields of the films-substrate system at different deposition temperatures: (a) 300 °C; (b) 350 °C; (c) 400 °C; (d) 450 °C.

B. Cooling Velocity Analysis.

The cooling velocity of films sputtered by PVD techniques depends on the cooling units equipped by sputtering chambers. Fig.3 depicts the thermal stress through the thickness of films-substrate system with different cooling velocities. It can be stated that there is a less effect of the cooling velocity on thermal stress on the edge of films-substrate system. For example, the maximum stress presented in each film with different cooling velocities varies less than 600 MPa. A slight variation of the stress for a relatively increase in cooling velocity can be accounted for that the stress is easy to relaxed on the edge, where the boundaries of films-substrate system are in free state. On the contrary, the cooling velocity influences the stress distributed on the center of combinatorial component significantly, and it is perceived in Fig.4. The maximum stresses of the films cooled down with different velocities vary in a considerable range. The possible reason is that the large strain appears on the center where the freedom is restricted by around areas and that is hardly accomplished, and subsequently the stress concentration is generated. Hence, the effect of changing the cooling velocity is mostly felt on

the thermal stress distributed on the center of films-substrate system.

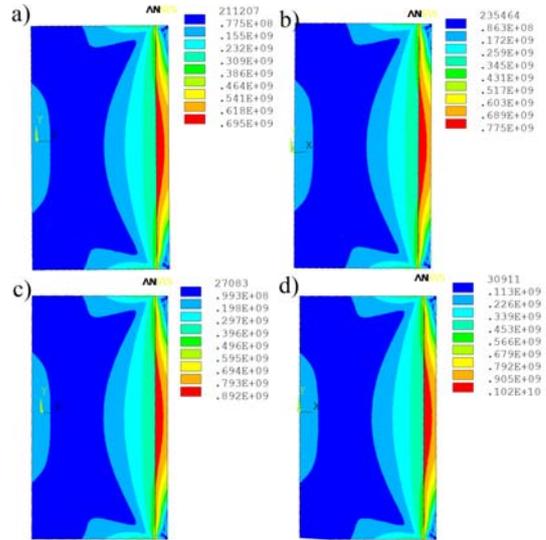


Fig.3 Thermal stress fields of the films-substrate system at various cooling velocity: (a) 0.5 W/(m²·°C); (b) 1.5 W/(m²·°C); (c) 2.5 W/(m²·°C); (d) 3.5 W/(m²·°C).

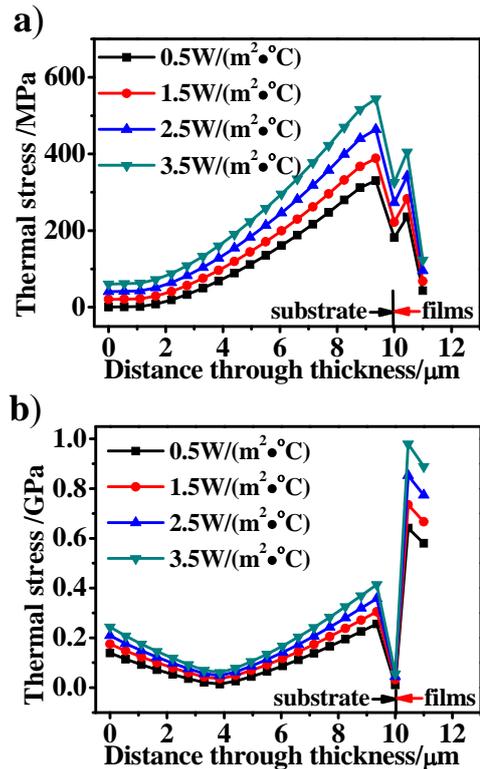


Fig.4 Thermal stress distribution through the thickness of films-substrate system with various cooling velocities on the (a) edge; (b) center.

IV. CONCLUSION

The influence of deposition temperature and cooling velocity on thermal stress generated in sputtered TiB₂ films during the films cooled down was investigated by finite element analysis codes. The stress increased because the bending strain caused by the rising of deposition temperature and cooling velocity added. As the strain can be easy to relax on the edge of films-substrate system with the same technical parameters, the stress distributed on the edge is lower than that on the center. Furthermore, the maximum stress appeared on the edge of films-substrate system with the deposition temperature and cooling velocity of 450 °C and 3.5 W/(m²·°C), respectively.

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