NUMERICAL SIMULATION FOR MEASURING YIELD STRENGTH OF THIN METAL FILM BY NANOINDENTATION METHOD①

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ABSTRACT The indentation process of aluminum film/silicon substrate combination by a rigid spherical indenter has been simulated using finite element method (FEM). It is demonstrated that both the yield strength and hardening index of the film affect the load-displacement curve. An empirical relationship among the strength parameters and hardness of the film has been established from the FEM results. Utilizing the relationship and the hardness measured by nanoindentation test for two different indentation depths, the yield strength and plastic hardening index of the film can be estimated.

Key words nanoindentation method thin metal film mechanical properties finite element method

1 INTRODUCTION

In integrated circuits (IC), aluminum and its alloy have been the most widely used materials for thin interconnect film. Because the thin film has thickness usually on the micrometer or submicrometer scale, the mechanical properties of the materials may be very different from those of their bulk materials. As the circuit densities of IC circuits have continually increased, more strict requirements for mechanical properties of thin film such as strength, thermal fatigue and stress relaxation have been proposed. In recent years, several experimental techniques to determine the properties of thin film have been developed. The most important of these is the nanoindentation test. The hardness and modulus of thin film on substrate have been a topic of interest in previous work[1, 2]. On the contrary, less study has been done for the fundamental mechanical properties such as yield strength and plastic hardening index, which play important roles in the failure of microelectronic device and the selection or optimization of the thin film technology[3, 4].

In this paper, the finite element method (FEM) is used to simulate the indentation process of Al film on Si substrate by a rigid spherical indenter, and the effect of the properties of Al film on the load-depth curves of indentation is demonstrated. Finally, a method for determining the yield strength and hardening index of the film is presented.

2 FINITE ELEMENT MODEL

The indentation problem is inherently one involving large deformations, particularly under the indenter where material of film may be displaced some distance. The material, geometric and contact conditional nonlinearities are needed to consider in the finite element model. The basic incremental equation used in FEM for large strain of elastoplasticity can be described as[5]

$$([K^s] + [K^f])\{\Delta\phi\} = \{\Delta p\} \qquad (1)$$

where $[K^s]$ is the elastoplastic stiffness matrix involving material nonlinearity for small strain, $[K^f]$ is the initial stress stiffness matrix involv-

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ing geometric nonlinearity for large strain, $\{\Delta \phi\}$ and $\{\Delta p\}$ are the incremental nodal displacement and load vectors, respectively. The nonlinear problem can be solved by Newtow-Raphson interative method for each displacement increment. A particular FEM procedure to large strain of elastoplasticity for indentation problem has been programmed. In this program, we assume that the spherical indenter is rigid, that the film and substrate are homogeneous, isotropic, and power-law hardening, and that the plastic response of the material is governed by Von Mises yielding criterion and isotropic hardening rule. We also assume that the film/substrate interface maintains perfect integrity, and that the indenter/film interface is frictionless. Additionally, axisymmetric properties are used to simplify the problem of indentation. Fig. 1 shows the finite element mesh for film and substrate. To simulate the indentation process, only the basic mechanical property parameters for the film and substrate are needed to input the program.

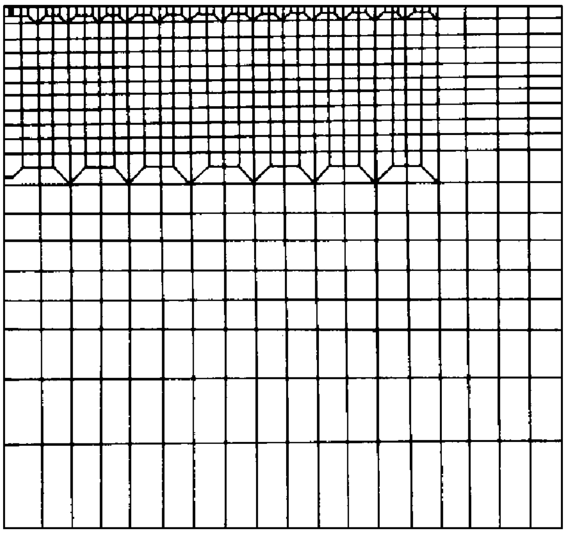

Fig. 1 Mesh for thin film and substrate

In order to confirm the validity of this program, the indentation process of Al film/Si substrate by a rigid conical indenter has been simulated, and the load-depth curve is compared with that calculated by Laursen *et al*[6]. In these two caculations, the material parameters are the same. Fig. 2 shows the two results and demonstrates that the precision of the present FEM analysis is sufficient. In the calculation, the indenter is treated as a cone having a perfectly sharp tip, and this is different from actual test conditions in which the indenter tip has a finite radius, thus giving rise to a different response. For this reason, a spherical indenter with a radius of 50 μm is used in the following calculations. The film thichness used in calculation is 1 μm and the maximum depth of indentation is equal to 0. 25 μm. The material properties are presented in Table 1, where the values of yield strength and hardening index are variable.

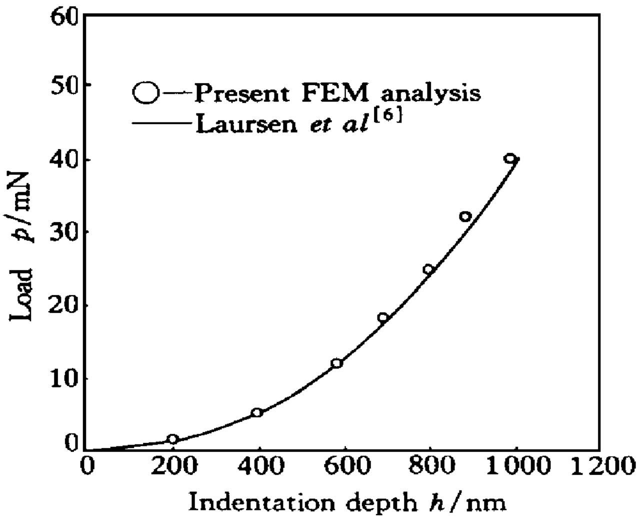

Fig. 2 Comparison between results from present FEM analysis and those from Laursen *et al*[6]

Table 1 Material properties

Material	Young's modulus /GPa	Poisson's ratio	Yield strength /MPa	Hardening index
Aluminum	76	0. 33	100~ 500	0~ 0. 15
Silicon	127	0. 28	4 410	0

3 RESULTS AND DISCUSSION

From the calculation of FEM, we can obtain much important information such as the load-depth curves of indentation, the elastoplastic stress or strain distributions, and the surface deformation of the film. In this paper, we concentrate on analyzing the effect of the mechanical properties of the thin film on load-depth curve, and the other problems will be discussed in another paper.

Fig. 3(a) (curves 1, 2, 3) shows the calculated load-displacement response in cases in which the yield strengths of the film are different but the strain hardening indices are the same. Similarly, Fig. 3(b) (curves 4, 5, 6) shows the response in cases in which the strain hardening indices of the film are different but the yield strengths of the film are the same. Obviously, the yield strength σ_{yf} of the film has qualitatively significant effect on the load response. As expected, for the film with a higher yield strength the load response is also larger, and the load difference for the films with different yield strengths remarkably increases with the indentation depth. In this reason, it is possible to determine the yield strength of the film through combining FEM and indentation method. As for the strain hardening index, it plays a similar role in load response to the yield strength. In the case that one of the two parameters (yield strength and hardening index) is known, the other can be determined easily by comparing the load response of calculation with that of indentation experiment. Unfortunately, both parameters are unknown and need to be determined. To do this, a method is presented below.

As the hardness testing techniques by nanoindentation method is gradually perfect, it is expected that the yield strength and hardening index of the film can be identified by the hardness. For the spherical indenter, the hardness of the film can be measured by nanoindentation method whose principle is similar to Brinell's. From a variety of results calculated by FEM, an empirical equation to describe the relationship among the yield strength, hardening index and hardness of film can be expressed as

$$\sigma_{yf}^{(1-n_f)}(S \cdot E_f)^{n_f} = K \cdot H_f \qquad (2)$$

where σ_{yf}, n_f are the yield strength and hardening index of the film, E_f, H_f the Young's modulus and hardness of the film, S, K the coefficients related to indentation depth. In this study, two different depths are considered. For the depth of 0.15 μm, S_1, K_1 are approximately equal to 0.09 and 3.17, respectively, and for the depth of 0.25 μm, S_2, K_2, 0.15, 3.0, respectively. The range of permitted variation for the material properties are: 100 MPa $\leqslant \sigma_{yf} \leqslant$ 500 MPa, $0 \leqslant n_f \leqslant 0.15$, and within the range there exists a good agreement between the given hardness and that from FEM calculation in which the material parameters (σ_{yf} and n_f) are determined by eq. (2) and the given hardness. Table 2 lists the comparison between calculated hardnesses and given hardnesses for an indentation depth of 0.25 μm.

The empirical eq. (2) is also examined by comparing the yield strength from Laursen *et*

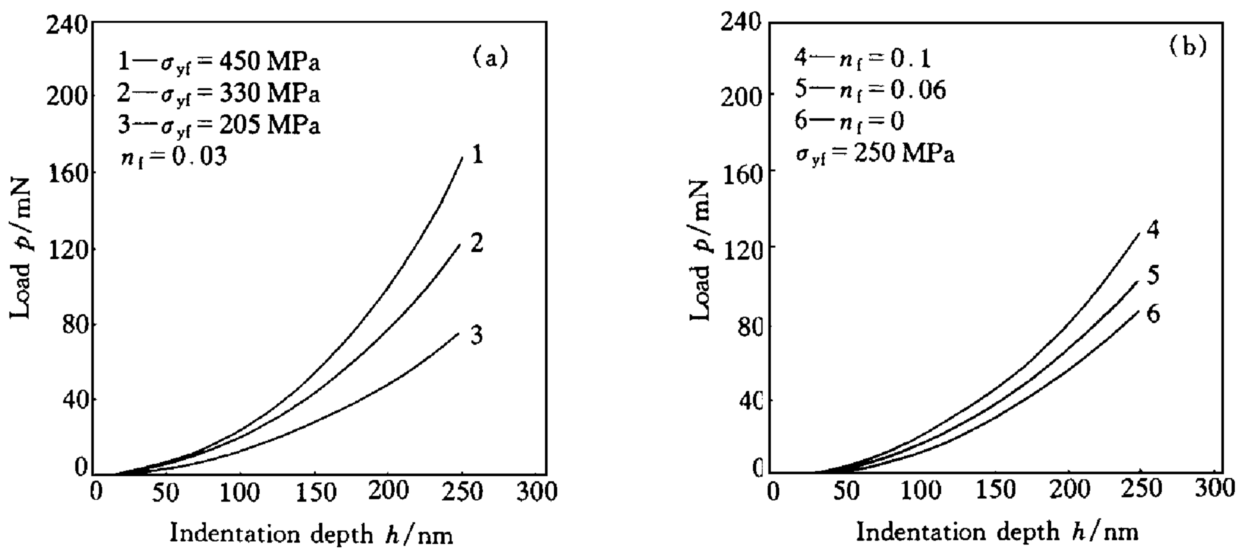

Fig. 3 Effects of yield strength (a) and hardening index (b) of film on load-displacement curves

Table 2 Comparison between calculated hardness and given hardness

Given hardness	Calculated hardness		
	$n_f = 0.03$	$n_f = 0.1$	$n_f = 0.15$
76	77.4	78.6	79
120	117.8	118.3	120.7
164	165.6	166.3	168.4

al[6] with that determined by eq. (2) from hardness. In the work of Laursen *et al*, they used a conical indenter and the material parameters which are the same as those in present analysis except for the yield strength being 485 MPa and the linear hardening modulus being 146 MPa. For the two indentation depths of 0.15 μm and 0.25 μm, the calculated hardnesses of Al film/Si substrate are almost the same, approximately 150. To substitute the hardness 150 and hardening index 0.01 (corresponding to the linear hardening modulus of 146 MPa) into eq. (2), we can determine the yield strength of the film. For the indentation depth of 0.25 μm, the yield strength is 435.6 MPa, and for 0.15 μm, it is 462.9 MPa. Obviously, there are some differences between the yield strength given by Laursen *et al* and that determined from eq. (2), and the difference decreases with the indentation depth. This can be attributed to the difference in the effect of substrate on the hardness which is calculated using different indenter shapes. For the same conditions, the plastic zone in the film under a spherical indenter is larger than that under a conical indenter, correspondingly, the effect of substrate on the hardness is also larger. So the yield strengths determined from eq. (2) are smaller than the given value when we use the hardness calculated for a conical indenter. Furthermore, the effect of substrate on hardness decreases as the indentation depth of a spherical indenter decreases, and this renders the yield strength determined from eq. (2) closer to the given value for the less indentation depth.

In order to determine the yield strength σ_{yf} and hardening index n_f of the film from the hardness, the coefficients S_1, K_1 and S_2, K_2 may be substituted into eq. (2) respectively, then an expression can be obtained by division as follows

$$\left(\frac{S_1}{S_2}\right)^{n_f} = \frac{K_1 \cdot H_{f1}}{K_2 \cdot H_{f2}} \tag{3}$$

Thus, the hardening index n_f of the film can be described as

$$n_f = \ln[K_1 \cdot H_{f1}/(K_2 \cdot H_{f2})]/\ln(S_1/S_2) \tag{4}$$

Using eq. (2) and eq. (4), the yield strength σ_{yf} of the film can be expressed as

$$\sigma_{yf} = \left[\frac{K_1 \cdot H_{f1}}{(S_1 \cdot E_f)^{n_f}}\right]^{\frac{1}{1-n_f}} = \left[\frac{K_2 \cdot H_{f2}}{(S_2 \cdot E_f)^{n_f}}\right]^{\frac{1}{1-n_f}} \tag{5}$$

where H_{f1}, H_{f2} are the hardnesses for the indentation depths of 0.15 μm and 0.25 μm, respectively. They can be obtained by nanoindentation tests with high precision. Finally, the hardening index and yield strength of the film can be determined from the measured hardnesses using eq. (4) and eq. (5).

REFERENCES

1 Fabes B D, Oliver W C, Mckee R A *et al*. J Mater Res, 1992, 7: 3035– 3064.

2 Pharr G M, Oliver W C, Brotzen F R. J Mater Res, 1992, 7: 613– 617.

3 Bader S, Kalaugher E M, Arzt E. Thin Solid Film, 1995, 263: 175– 184.

4 Shute C J, Cohen J B. J Mater Res, 1991, 6: 950– 956.

5 Meng F Z. The Finite Deformation Theory and Finite Element Method for Elastoplastic Problem, (in Chinese). Beijing: Qinghua University Press, 1985.

6 Laursen T A, Simo J C. J Mater Res, 1992, 7: 618 – 626

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