Extended Abstracts of the 2006 International Conference on Solid State Devices and Materials, Yokohama, 2006, pp. 494-495

P-2-17

Finite element analysis of nanometer-scale contact for low temperature bonding

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1. Introduction

Surface activated bonding (SAB) is a method for low temperature bonding utilizing attractive forces between atomically clean surfaces [1]. The clean surfaces are obtained by dry etch process such as the bombardment of Ar fast atom beam or ion beam, or plasma irradiation. Since the bonding takes place at the contact area between the two surfaces, the real area of the contact and the deformation of the area determine the characteristics of SAB. Recent studies of the room temperature bonding of silicon and copper showed that the surface roughness in a nanometer-scale range influences critically the bond strength. Experimentally the surfaces with a surface roughness lager than 3 nm Ra can not be bonded at room temperature, whereas the surfaces of smaller than 3 nm Ra can be bonded under a certain compressive pressure [2]. Such effects of the surface roughness on the bond strength have been explained by simple elastic contact models. Takahashi [3] calculated local deformation simply by considering the van der Waals forces acting between semicircular surfaces of elastic continuous body. According to the model, the necessary condition of a full contact of the surfaces is that the elastic strain energy per unit area is equal to or less than the work of adhesion $\Delta\gamma$. In case the surface asperity is approximated by a sine wave, the condition for the full contact is described as follows.

$$\frac{h^2}{L} \leq \frac{4(1-\nu^2)}{\pi E}\Delta\gamma = 0.013nm \qquad (1)$$

where E is young's modulus, and ν is Poisson's ratio. When wave length L=70nm, the condition of amplitude h is described as follows.

$$h \leq 0.95nm$$

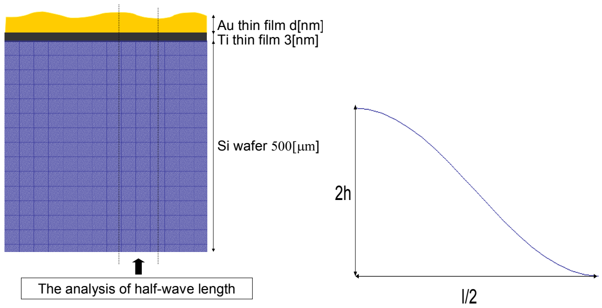
However the real bond strength is not likely to be determined only by the contact area. A common observation is that once bonding is succeeded, the measured bond strength often is not dependent of the bonded area, but rather so strong that the bond strength can not be measured by fracture test, because the failure does not occur in the bonded interface but always a bulk failure in the bonded materials is observed.

The influence factors of the bond strength which have not been incorporated in the previous elastic theory are the plastic deformation and the residual stresses in the vicinity of the bonded interface in nanometer-scale.

In this paper, FEM analysis of the contact process is investigated for bonding Au thin films on Si wafers with nanometer-scale roughness. The influence factors to the contact ratio and the stress distribution are clarified quantitatively in terms of the applied load σ_{cont} for the full contact and the residual stress distribution.

2. Contact analysis model using FEM method for elasto-plastically deformed asperities

Fig. 1(a) shows Au thin film on Si wafer for the FEM models. FEM analysis was carried out using the software ANSYS9.0 under two dimensional plane stress condition. The surface asperity was approximated by a sine wave as shown in Fig. 1(b). According to the SAB principle, it is assumed that contact surfaces are adhered with the coefficient of friction of ∞, once they come into contact. Fig. 2 shows the FEM model and mesh used in the calculation. The contact of Au thin films is analyzed equivalently to the contact of the Au thin film to the rigid body. The model is axisymmetric; thus only a half-wave length is analyzed. Each material is elasto-plastic material with a bilinear isotropic-hardening behavior.



(a) (b)

Fig. 1 (a) Au thin film on Si wafer
(b) Sine wave approximating surface asperity

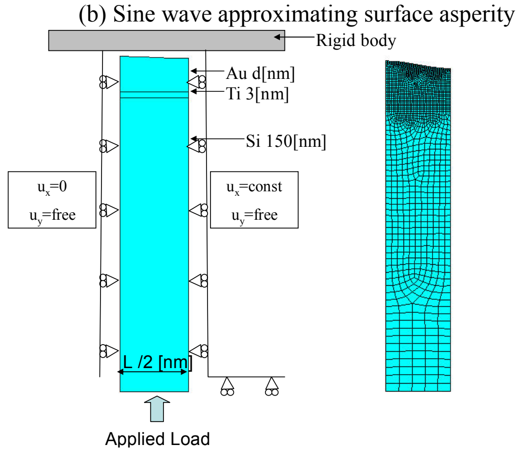


Fig. 2 FEM model and mesh used in the calculation

3. The effect on contact process by difference of scale

Three models were analyzed with an entire scale multiplied by 1x, 10x, 100x, assuming h=1.0nm (on scale

1x). The ratio of the contact over the projection area was calculated for each model for various values of applied loads. The contact ratio is almost the same for different scale as shown in Table I. This result means that the scale effect of plastic deformation is very small.

Table I Contact ratio for scale analysis

Applied Load [MPa]	Scale 100 x	Scale 10 x	Scale 1 x
0	0.0071	0.0071	0.0071
400	0.3134	0.3134	0.3134
800	0.5489	0.5562	0.5562
1200	0.7777	0.7777	0.7778

4. Applied Load for the full contact

As mentioned in the previous section, the compression process of surface asperity is independent of the model scale, even it is an elasto-plastic analysis. Therefore, the two independent factors of L/h and L/d control the compression process, and determin the maximum contact stress σ_{cont} for the contact ratio of 1. Fig. 3 shows the relationship of σ_{cont} vs. h/L. σ_{cont} increases in the logarithm over h, while gradually to d, because the contribution of the plastic deformation is not so large. Fig. 4 shows the condition of the full contact in respect of the wave length L and roughness h for various applied load and for van der Waals force calculated by Eq.(1). This result shows that van der Waals force is predominant compared with the external load in the area where the surface roughness is small, and the aspect ratio is high, and vice versa.

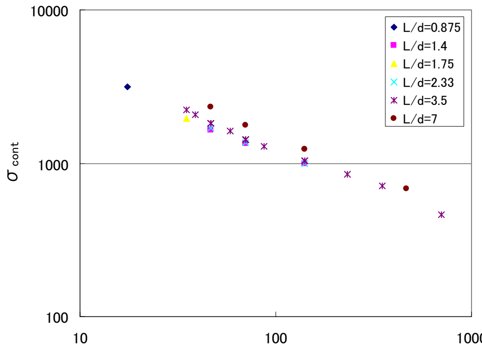


Fig. 3 Maximum contact stress σ_{cont} vs. h/L

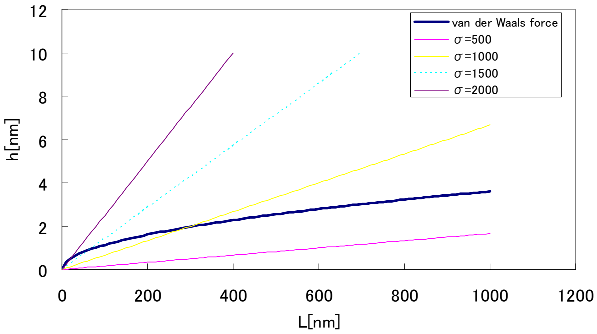


Fig. 4 The condition for the full contact by external load and van der Waals force

5. The analysis of residual stress

Fig. 5 shows the residual stress distribution in term of equivalent stress after the external load is removed in case of h=1.0nm, L=70nm, d=20nm, σ=400MPa. It is clear that the residual stress value becomes maximum on the edge of the contact area.

Fig. 6 shows the relationship between the maximum value of the residual stress and the contact ratio. It turned out that the maximum residual stress is saturated to a maximum value when the contact ratio becomes more than 0.5.

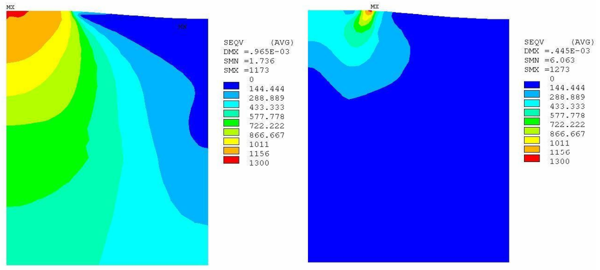


Fig. 5 Equivalent stress under the external load (left) and the residual stress after the release of the load (right)

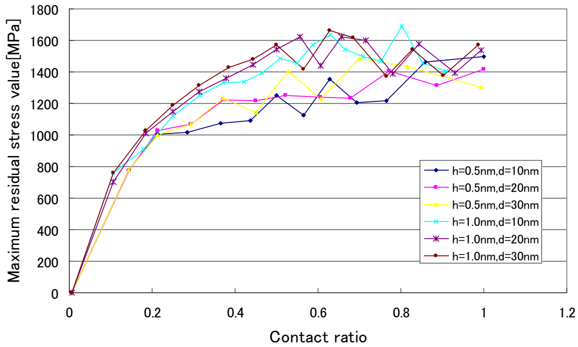


Fig. 6 The maximum residual stress vs. contact ratio

6. Conclusion

The contribution of the van der Waals forces to the full contact is dominant for the large wave length of the roughness. The plastic deformation in nanometer scale is not relevant to the ultimate contact. The saturation of the residual stress over the contact ratio more than 0.5 may explain the experimental observations that an interfacial failure occurs in the large range when bond strength is small, while the bonding remains kept on all the contact area if the failure does not ever occur.

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