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EFFECT OF SURFACE ROUGHNESS ON THE ADHESION OF SILICON WAFERS PRIOR TO BONDING

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To understand the effect of surface roughness on silicon wafer bonding, a continuum mechanical model is presented. This model is based on Obreimoff's experiment and the contact theory of rough surfaces. The surface energy of silicon was calculated to be much reduced than the theoretical value. Problems are discussed concerning surface film effects and the assumption of constant asperity radius and statistical distribution function.

INTRODUCTION

The understanding of the basic science of silicon wafer bonding is still lacking, despite significant progress having been made in optimizing the bond process (1). Bond strength critically depends on the initial surface preparation and the temperature history of the joined wafers. It is, therefore, important to study the initial bond strength before heat treatment under various conditions including variations of surface roughness, flatness, surface chemistry, crystallography and surface defects. While surface roughness effects are very important in controlling the adhesion bond strength of various materials such as glass and rubber (2), there has been no systematic study of the effects of surface roughness on the characteristics of silicon wafer bonding.

The adhesion of two bodies can be described by continuum theories. These macroscopic models do not require any specific type of force. Therefore, by using macroscopic models, one can calculate the adhesion force or energy without knowing the type of force acting between two surfaces. Hertz (3) proposed a model explaining contact behavior between two rigid spheres, assuming no adhesion between them. Johnson *et al.* (4) has modified the Hertz model to incorporate the adhesion force between two spheres. Fuller and Tabor's model (2) developed this for contacting surfaces, and surface profiles are regarded as random signals which make contact where they would otherwise overlap.

The objective of this research is to study the effects of surface roughness on the initial bonding strength of hydrophilic wafers before heat treatment. Using Fuller and Tabor's contact theory (2) and the force-crack geometry relation in Obreimoff's experiment (5), a model is developed to relate the bond energy as a function of surface roughness to the work done to separate a bonded wafer pair, by which the adhesion energy of contact can be estimated.

EXPERIMENTAL

Silicon wafers were cleaned following standard RCA cleaning procedures in a cleanroom. After the cleaning procedure, the wafers were etched in a solution mixture of H_2O, H_2O_2 and NH_4OH. To increase the surface roughness, higher concentrations of NH_4OH than the normal RCA 1 cleaning solution were used. Surface roughness was measured by atomic force microscopy. A special set up was devised to measure the crack propagation length at the interface according to the razor-blade insertion method as shown in Fig. 1.

THEORY

In the frictionless contact of elastic solids, the contact stress depends only on the relative profile of their two surfaces, i.e. the gap between them before loading. The system may then be replaced by a flat, rigid surface in contact with a body having an effective modulus E* and a profile which results in the same undeformed gap between the surfaces. We are concerned here with the contact of two nominally flat surfaces, which have r.m.s.

roughnesses σ_1 and σ_2 respectively. However we shall consider the contact of a rigid flat plane with a deformable surface of equivalent roughness $\sigma = (\sigma_1^2 + \sigma_2^2)^{1/2}$.

The situation is illustrated in Fig. 2. We shall follow the analysis of Fuller and Tabor (2). After the surfaces have been compressed to a minimum separation d_0, if the separation is increased, the total contact force between the two surfaces (2) will be

$$P = \frac{Np_c}{(2\pi)^{1/2}} \int_{-Lo}^{\infty} F\left(\frac{\Delta}{\Delta_c}\right) \exp\left\{-\frac{1}{2}(h+\Delta)^2\right\} d\Delta, \quad [1]$$

where $\Delta = \delta/\sigma$, $\Delta_c = \delta_c/\sigma$, $h = d/\sigma$, and the limit of integration $Lo = \Delta_c$ or $(h - h_0)$, whichever is the less. σ is the standard deviation of asperity heights, δ is the displacement of their tips relative to the undeformed part of the plane, and d is the separation between planes. δ_c represents the maximum extension of tip of an asperity above its undeformed height before separation occurs. N represents number of asperities per unit area and the maximum force which can be sustained by adhesion before separation is p_c.

As the separation is increased from $h = h - h_0$ the force between surfaces becomes tensile, reaches a minimum value ($-P_m$) and then tends asymptotically to zero as the adhesion between the highest asperities is finally broken. P_m is the 'pull-off force' for the whole surface as compared with p_c for an individual asperity. The ratio P_m/Np_c expresses the reduction in adhesion due to the dispersion in the asperity heights.

The strength of the bond created during contact at room temperature can be measured quantitatively by a razor-blade insertion method developed by Maszara *et al.*(6) which is based on a theoretical analysis of Obreimoff's experiment (5) by Gillis and Gilman (7,8). This theory predicts the following relationship between the surface energy and the geometry of a crack :

$$\gamma = \frac{3Et^3y^2}{8L^4} \quad [2]$$

where γ is the specific surface energy, $2y$ and L are the crack separation and length, respectively, t is the thickness of the wafer and E is the modulus of elasticity. Because Eq. 2 assumes a perfectly smooth surface, it gives a very low bonding energy due to the falsely exaggerated contact area. Instead of using Eq. 2, one can apply Eq. 1 to the calculation of bonding energy.

Because P is a function of the surface roughness, the number of asperities, the mean radius of asperities, and the surface energy, if we can derive a relationship between force and the crack geometry from Obreimoff's experiment (7), and substitute this relation with P (total contact force) in Eq. 1, the surface energy can be calculated in terms of the surface roughness and the crack geometry. If the propagation of the crack is reversible, the energy balance for creating new surfaces is given by

$$dW = dU + dS, \quad [3]$$

where dW is the work done when the crack length increases by dL, and dU is the increase in strain energy, and dS is the energy of the newly created surfaces. The incremental work is

$$F dy = \frac{F^2L^2}{EI} dL. \quad [4]$$

The bending moment of each beam is $M(x) = Fx$, and the strain energy U due to this bending moment in each beam is

$$U = \frac{1}{2EI} \int_0^L M^2(x) dx = \frac{F^2L^3}{6EI}. \quad [5]$$

The incremental strain energy is

$$dU = \frac{F^2L^2}{2EI} dL = \frac{dW}{2}, \quad [6]$$

where I is the moment of inertia ($=\omega t^3/12$), F is the force applied, $2y$ is the thickness of the deflection, ω is the width of the cantilever, and L is the length of the cantilever beam. The specific surface energy is given by

$$dS = \gamma\omega dL \quad [7]$$

By substitution of the above equations into Eq. 3, we have

$$S = 3U \qquad [8]$$

or

$$\gamma = \frac{6F^2L^2}{E\omega^2t^3}. \qquad [9]$$

From Eq. 9, one can determine the force required to separate a bonded silicon wafer pair from the crack length using the razor-blade insertion method. This force is essentially the same as the total contact force, P, in Eq. 1. Since we are dealing with the maximum pull-off force, Eq. 1 can be rewritten

$$\frac{E\gamma wt^3}{4L^3} = \left(\frac{P_m}{Np_c}\right)Np_c \qquad [10]$$

When all surface topographic parameters are known, such as the mean asperity radius, the number density of asperities, surface roughness and the crack geometry, the surface energy can be determined from the above equation by an iteration method or a graphical solution.

RESULTS AND DISCUSSION

Fig. 3 shows theoretical relationship between the normalized force and the normalized separation for the adhesion of two silicon surfaces. Note that these are the force-separation curves as the separation between the two surfaces is increasing. Young's modulus of silicon was taken as 131 GPa, and the Poisson's ratio as 0.279. Surface energy was taken to be 1.4 J/m^2 from the literature (9). Mean asperity radius of 240 Å was used for the calculation purpose. The maximum tensile force or pull-off force, P_m, can be determined as a general function of Δ_c by carrying out a whole series of similar computations. This is shown in Fig. 4 where the vertical axis is P_m / Np_c and the horizontal axis is $1/\Delta_c$. Since

$$1/\Delta_c = \sigma/\delta_c = \frac{1}{3\beta}\left(\frac{3\beta p_c}{K}\right)^{\frac{2}{3}}, \qquad [11]$$

$$p_c = \frac{3}{2}\pi\beta\Delta\gamma., \qquad [12]$$

Δc is directly proportional to surface roughness, σ. The relationship between Δc and σ can be easily found using this equation, and shown in Fig. 4. The results of the present analysis shows that, if the surface roughness of silicon wafers exceeds 7 Å, they will not bond together. For the surfaces with surface roughness of less than 1 Å, more than 90% of normalized force can be obtained.

RCA1-prepared silicon surface has a surface roughness of 0.79 Å. After the etching process, surface roughness becomes 3.24 Å. The asperity radius and the number density of the asperities are also varied according to the concentration variations of NH_4OH. Surface characterization results are summarized in Table 1.

When Eq. 2 is used for the surface roughness of 3.24 Å, a surface energy of 0.240 J/m^2 and a contact force per unit area(m^2) of 1600 J/m are obtained as shown in Table 1. Fig. 5 shows the surface energy effect on the normalized force plotted against the normalized separation for the contact between surfaces with various surface energies for surface roughness of 3.24 Å. Fig. 6 shows the relationship between the maximum pull-off force, divided by Np_c, and surface energy for the surfaces of roughness 3.24 Å. Because this curve corresponds the right hand term of Eq .10, this should also be equal to the left hand term, that is, the total contact force per unit area, in Eq. 10 at a specific surface energy. This specific surface energy is the 'true surface energy' as shown in Table 1.

The reported surface energy for a clean, untreated surface of silicon is 1.4 J/m^2, but the calculated surface energy of the hydrophilic silicon wafer is 0.282 J/m^2, while the apparent surface energy obtained from Eq. 2 is 0.240 J/m^2. In Eq. 2, the crack geometry parameters such as the crack propagation length already contain the surface roughness effect, therefore, using Eq. 2, one cannot separate the 'true' surface energy from the 'apparent' surface energy. Because, in Eq. 10, there is a surface roughness term, it should give a surface energy value similar to the theoretical surface energy of silicon, that is, 1.4 J/m^2.

This discrepancy can be explained in several ways. One is that it is not reasonable to expect a theoretical surface energy from Eq. 10 in the case of hydrophilic silicon wafer bonding. A hydrophilic wafer surface has Si dangling bonds joined to OH groups and thus its surface

energy is expected to be considerably lower than the calculated value for an exposed silicon surface in vacuum. Indeed, calculations of hydrogenated Si surfaces show a considerable reduction in surface energy (10).

Other possibilities can be found in the basic assumptions in Eq. 10. This assumes only elastic deformation and does not deal with plastic deformation or viscoelastic effects. Furthermore, it also assumes that a rough surface consists of asperities with various heights but with the same asperity radius. To solve this problem, one can use a modified distribution function which incorporates asperity radii rather than following the one Fuller and Tabor used. Finally, Np_c is the pull-off force for a surface consisting of asperities all of the same height, and this is the consequence of modeling a rough surface by discrete asperities that are assumed to deform independently of each other and have tips all of the same radius. This model will be developed further to include more realistic assumptions of surface topography.

CONCLUSIONS

As a conclusion, a model was developed to overcome the problems of measuring surface energy. This is based on a contact model between a rigid plane and a rough surface. The advantage of this model is that the surface roughness effect on the adhesion strength can be easily understood. For normal silicon wafers, even if the surface energy is the same as the reported value, the wafers will not bond together when their surface roughness is more than 7 Å. The calculated surface energy from this model is 0.282 J/m^2 for a bonded wafer pair when surface roughness is 3.24 Å. There is a significant gap between the reported surface energy and this surface energy value. The main reason for this difference is attributed to the presence of OH bonds at the interface which affect the surface energy.

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Table 1 Surface treatment condition, surface characterization result and surface energy calculation result.

H_2O:H_2O_2:NH_4OH	5:1:3
Etching time	50 min
Etching temperature	75 °C
Surface roughness (Å)	3.24
Asperity density (μm^2)	1800
Asperity radius (Å)	240
Apparent surface energy (J/m^2)*	0.240
True surface energy (J/m^2) **	0.282

* calculated from Eq. 2
** calculated from Eq. 10

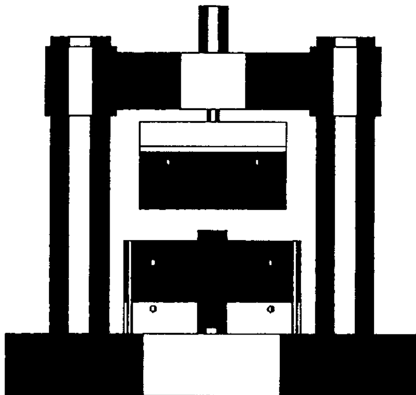


Fig. 1 Experimental setup for measuring surface energy.

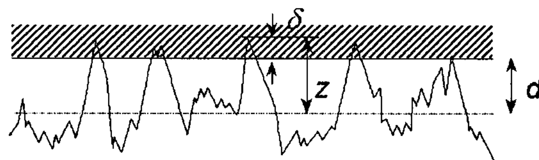
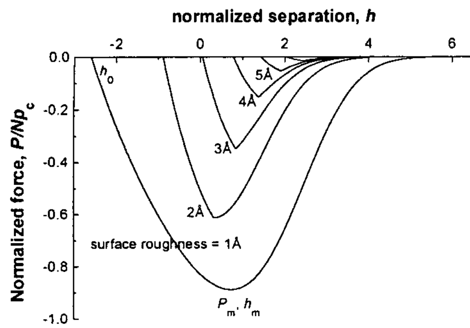


Fig. 2 Contact of a randomly rough surface with a smooth flat surface.



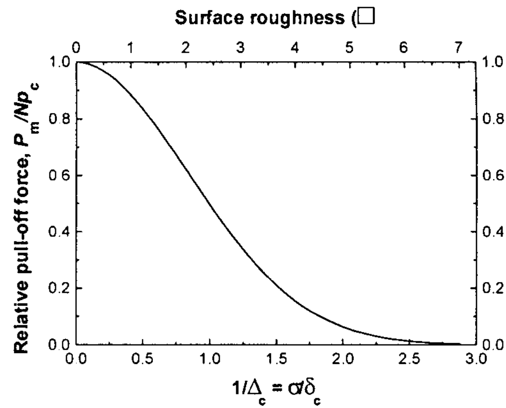
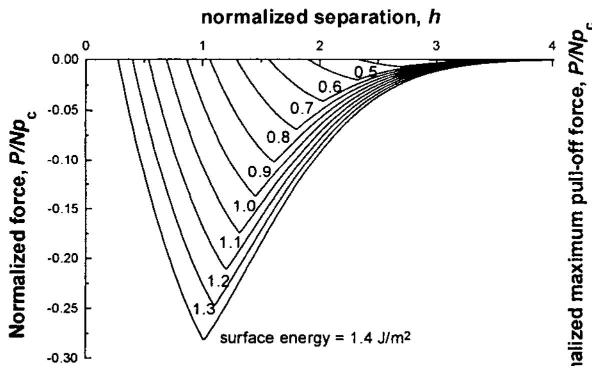


Fig. 3 Theoretical relationship between the normalized force and the normalized separation for the interface separation of bonded wafer pairs.

Fig. 4 Relative pull-off force plotted against surface roughness and $1/\Delta_c$.



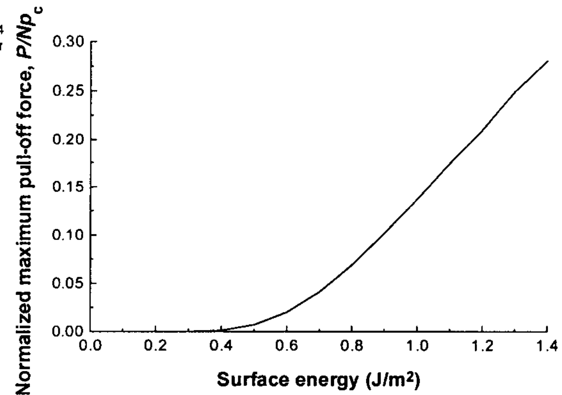


Fig. 5 Force-separation curves for silicon wafers with various surface energies. (surface roughness = 3.24 Å, asperity density = $1800/\mu m^2$, asperity radius = 240 Å)

Fig. 6 Relative pull-off force plotted against surface energy for a silicon wafer pair.