Modeling the formation of spontaneous wafer direct bonding under low temperature

Zirong Tang *, Tielin Shi, Guanglan Liao, Shiyuan Liu

Wuhan National Laboratory for Optoelectronics, Wuhan 430074, China
State Key Laboratory of Digital Manufacturing Equipment and Technology, Huazhong University of Science and Technology, Wuhan 430074, China

ABSTRACT

Low temperature wafer direct bonding is one of critical technologies in micro/nano fabrication. In this study, a description of interfacial requirements for spontaneous wafer direct bonding under low temperature is proposed. The model relates the occurrence of bonding to interfacial adhesion energy, interfacial nano-topography and elasticity of wafers. Its derivation is based on Johnson–Kendall–Roberts (JKR) theory and a competition between the bonding energy and the deformation of interfacial micro/nano-roughness. The analysis identifies three bonding possibilities, namely spontaneous bonding without voids, spontaneous bonding with voids, and bonding under external pressure with gap or un-bondable. To verify the model, experiments were carried out for silicon wafers with different surface nano-scale roughness.

1. Introduction

Wafer bonding processes are widely developed and applied in semiconductor industry, from silicon-on-insulator materials to optoelectronic devices, but the bonding mechanisms remain poorly understood with regard to their interfacial nano-topography [1]. Due to stress-related reliability issues of high temperature, high pressure and bonding with intermediate layers involved in the bonding process, low temperature wafer direct bonding with spontaneous or self-propagating capabilities can find more industrial applications. Spontaneous wafer bonding is described as a special phenomenon from which the bonded area can be seen spread over the entire wafer surface, particularly for hydrophilic wafers bonding under low temperature (usually less than 200 °C). Interfacial properties of bonding pair will have direct effect on bonding results, and high surface waviness and roughness will result in failing to bond or bond with the formation of voids and gaps at the bonded interface [2]. Therefore, it is critical to understand spontaneous bonding mechanism, especially the formation mechanism with respect to the interfacial properties of bonding pair.

In the present, there are two major contact theories which consider the surface attraction forces between the contact surfaces, namely DMT (Deryagin, Muller, and Toporov) theory and JKR the-

ory [3]. Several groups have investigated the effect of interfacial properties on wafer bonding and surface contact mechanics of room temperature wafer bonding. In Farrens's work [4], a van der Waals force model is set up to model the initial contact bond force, while the model is the reliance upon quality information about the chemical nature and dielectric properties of activated bonding surface. In Bengtsson's study [5], a model based energy conservation is set up to explain why the contact wave velocity in silicon wafer bonding decrease with wafer thickness. In Yu's modeling [6], elastic accommodation is considered to bond the misfit wafers. Gui [7] studied the effect of surface roughness on wafer bonding based on DMT contact theory and made a statistical surface roughness model. They also conducted some experiments to bond silicon wafers with different surface roughness. It turned out that surface roughness had great effects on the bonding results. Reiche studied the bonding speed of silicon wafers in one work [8], it showed that the lateral bonding speed of room temperature bonded wafers increases with decreasing pressure, and is inversely proportional to the viscosity of the ambient gas. In his another work [9], the defect formation at bonded interface is studied through molecular dynamics simulation. However, the spontaneous phenomenon in wafer bonding was not considered in their work, the mechanism of spontaneous wafer bonding was not revealed yet up to now, and no quantitative model for this process exists to date.

In this study, we addressed the problem of spontaneous wafer bonding in relation with the properties of wafer surfaces under low temperature, and silicon wafers were used as an experimental model system. Since the surface of commercial wafer available was

* Corresponding author. Address: State Key Laboratory of Digital Manufacturing Equipment and Technology, Huazhong University of Science and Technology, Wuhan 430074, China. Tel.: +86 27 87792241; fax: +86 27 87792413.
E-mail address: zirong@mail.hust.edu.cn (Z. Tang).

sufficiently flat, only surface waviness and roughness were concerned in this work. Following JKR theory, a mathematical model was proposed to study the effect of nano-topography on bonding process and the formation of spontaneous wafer direct bonding under low temperature. In the end, experiments were also carried out and experimental results were analyzed to verify the model.

2. Theoretical analysis

Fusion mechanism was generally considered for high temperature wafer bonding (usually over 450 °C), while contact theory was applied for wafer direct bonding under low temperature. In the following, a contact model was developed first, then the conditions of spontaneous bonding was justified and the effect of surface roughness was discussed.

2.1. Model development

It was agreed that the JKR theory is valid for solids with a large surface energy [10], which is generally the case for hydrophilic wafer bonding because nano-scale roughness is in the range of nano-scale where the adhesion forces between contact solids are in a dominant position. According to the conclusion of Greenwood [11], the effect of model considered roughness on two surfaces is the same as the model assumed that one of the contact surfaces is perfectly flat, so here the lower wafer surface is assumed to be perfectly flat. Since the dimensions of the asperities on wafer surface are sufficiently small, the wafer bodies can be considered infinitely. Taking wavelength of asperity as a measure, the schematic drawing of model of low temperature wafer direct bonding was showed in Fig. 1. Assuming that the surface nano-scale profile of upper wafer are periodically rough, which could be given by $f(x) = h \sin^2\left(\frac{\pi x}{L}\right)$, where $x \in (kL - a, kL + a)$, $2a < L$, k is an integer, a is the radius of contact zones, L and h are the length and height of gap respectively. According to contact mechanics of periodically roughness surfaces [12], the pressure (line force, with a dimension of force/length) distribution underneath the asperities inside the contact zones can be deduced as the following:

$$p(x) = \frac{\cos\left(\frac{\pi x}{L}\right)}{\sqrt{\sin^2(\pi a/L) - \sin^2(\pi x/L)}} \left\{ \frac{E^* h\pi}{2L} [\sin^2(\pi a/L) - 2\sin^2(\pi x/L)] + \frac{F}{L} \right\}, \quad (1)$$
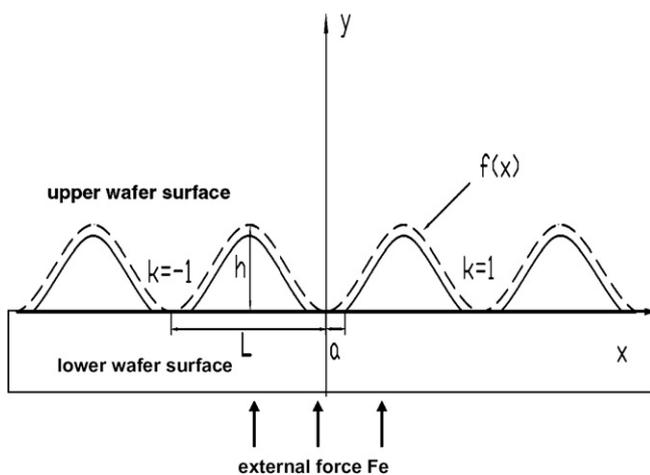

Fig. 1. Schematic drawing of nano-topography of the bonding interfaces, where dashed line represents interfacial geometry before bonding and solid line represents that after bonding.

where $E^* = \left(\frac{1-v_1^2}{E_1} + \frac{1-v_2^2}{E_2}\right)^{-1}$ is elastic modulus, E_i and v_i are Yong's modulus and Poisson's ratio respectively, F is the force per asperity on wafer surface, which is also a combined force of both adhesion force and external forces. In Hertz contact, there is no adhesion, the left side of Eq. (1) is equal to 0 when x → −a, then

$$\frac{E^* h\pi}{2L} \sin^2\left(\frac{\pi a}{L}\right) = \frac{F}{L} \quad (2)$$

where F is contributed by external force F_e, namely, Hertzian contact F is given by

$$F = \frac{E^* h\pi}{2} \sin^2\left(\frac{\pi a}{L}\right) \quad (3)$$

Assumed that the wafers contact fully, then $2a \to L$, the limit Hertzian contact force is

$$F_{lim} = E^* h\pi/2 \quad (4)$$

If the surface adhesion is taken into account, contact forces will be contributed by both the adhesion force and the external force F_e. According to JKR theory, the contact zone size $2a$ is determined by equating the energy release rate of the gap outside the contact zone ζ to the wafer surface energy W. Because the surface contact forces are assumed to act in a region of vanishing area, for surface profile given by $f(x)$, the energy release rate ζ is [11]

$$\zeta = \left(\frac{E^* h\pi}{2L} \sin^2 \frac{\pi a}{L} - \frac{F}{L}\right)^2 \frac{L \cot(\pi a/L)}{2E^*} \quad (5)$$

The relation between the contact zone size $2a$ and F is obtained by imposing the condition $\zeta = W$ and above equation becomes

$$F = \frac{E^* h\pi}{2} \sin^2 \frac{\pi a}{L} - \sqrt{2E^* W L \tan(\pi a/L)} \quad (6)$$

For better understanding the correlation between the surface energy and the surface profile, A dimensionless parameter is introduced as the following,

$$\hat{F} = \frac{F}{F_{lim}} = \sin^2(\pi c) - \alpha\sqrt{\tan(\pi c)}, \quad (7)$$

where F_{lim} is defined by Eq. (4), $c = a/L$, α is a dimensionless parameter defined as

$$\alpha = \frac{2\sqrt{2}}{\pi} \frac{\sqrt{L}}{h} \sqrt{\frac{W}{E^*}} \quad (8)$$

Fig. 2 plots the normalized force $\hat{F}$ versus the normalized contact length c for different values of α. The special case of $\alpha = 0$ corresponds to the Hertzian contact where there is no interfacial adhesion. According to Eq. (7), if $\hat{F}$ is positive, it means that external force is needed ($Fe > 0$) to bond wafers. With the increase of α, $\hat{F}$ is decreasing while c is kept constant, and if $\hat{F}$ is negative or zero for all $0 \leqslant c \leqslant 0.5$ it means that no external forces is needed for bonding, or it means that bonding will occur spontaneously.

According to Eq. (7), there is a maximum value $\hat{F}$ or $\hat{F}_{max}$ for each α at $0 \leqslant c \leqslant 0.5$. If $\hat{F}_{max}$ is positive, it means that external force is needed ($Fe > 0$) to bond wafers. With the increase of, $\hat{F}_{max}$ is decreasing, until $\hat{F}_{max} = 0$, a critical value $\alpha = \alpha^*$ can be calculated under this case, where $\alpha^* = 3^{\frac{3}{4}}/4 \approx 0.57$. When $\hat{F}_{max}$ is less or equal to zero all $0 \leqslant c \leqslant 0.5$, it means that no external force is needed for bonding. And for spontaneous bonding to occur with full contact or wafer self-propagating, it must also satisfy the condition $d\hat{F}/dc \leqslant 0$ for all $0 \leqslant c \leqslant 0.5$ which yields another critical value of α or α_c, which can be found to be $\alpha_c = \frac{15}{16}\left(\frac{5}{3}\right)^{\frac{1}{4}} \approx 1.065$. It means that the parameter α must be large enough to satisfy the condition of self-propagating wafer bonding without gap or voids. From Eq. (8), we can see that there are several ways of increasing the value of parameter α, such as increasing the surface energy of wafer or using wafers with the smaller surface roughness. Using the critical
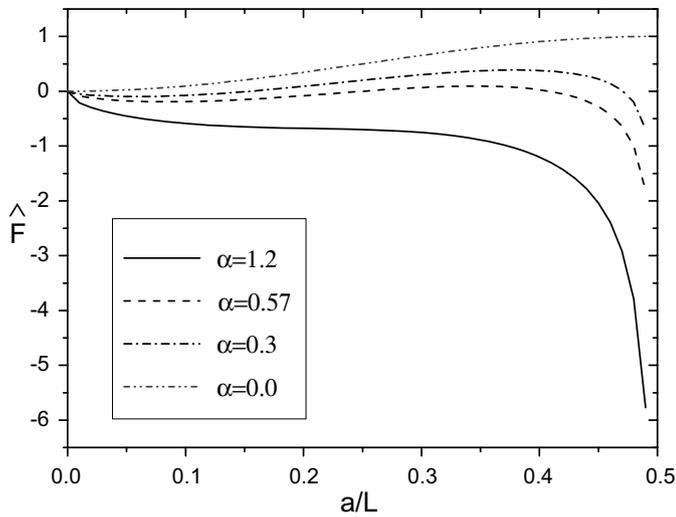
Fig. 2. The dependence of the normalized contact force $\hat{F}$ on a/L for different values of α.

value $\alpha_c = 1.065$, the critical condition for spontaneous wafer bonding can be obtained

$$h = \frac{1}{1.065} \frac{2\sqrt{2}}{\pi} \left(\frac{WL}{E^*} \right)^{\frac{1}{2}} \tag{9}$$

The above equation can be used to justify the formation of spontaneous wafer direct bonding under low temperature. As a special case, it will be used to analyze on silicon wafer direct bonding in the following section.

2.2. Effect of surface roughness on spontaneous bonding

Taking silicon direct wafer bonding as example, applying typical material parameters [7], surface energy of silicon wafer $W = 0.1$ J/m^2, Young's modulus $E = 160$ GPa, and Poisson's ratio $v = 0.28$, therefore we can get silicon elastic modulus $E^* = 70.53 \times 10^9$. According to Eq. (9), we plot gap height h against gap length L of silicon wafers for $\alpha = 0.57$ and $\alpha = 1.065$. Three regimes can be identified from Fig. 3. When gap height is less than the critical height of self-propagating, which is in the regime III, wafer would
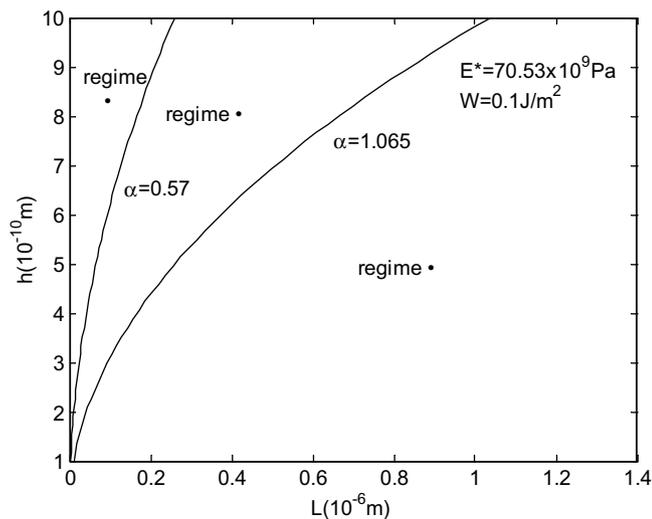
bond spontaneously without voids due to surface forces. When gap height exceeds the critical height of gap-closing that is in the regime II, voids would appear in wafer bonding. When gap height exceeds another critical value, which is in the regime I, voids will still exist even with external forces.

Considering the two critical value $\alpha = 0.57$ and $\alpha = 1.065$, we can plot the correlation of gap height h with wafer surface energies and the correlation of gap length L with wafer surface energies as shown in Fig. 4 and Fig. 5, respectively. The results showed that higher surface energy will render larger surface roughness, which was described by lower gap height and shorter gap length. This explained that the activation of wafer surface for bonding was another critical condition for formation of spontaneous bonding, and in the next section, experiments were designed with the activation of wafer surface before bonding.

3. Experimental results and discussion

To verify this model, we conducted experiments on silicon wafers with different surface roughness. The details of the experiment
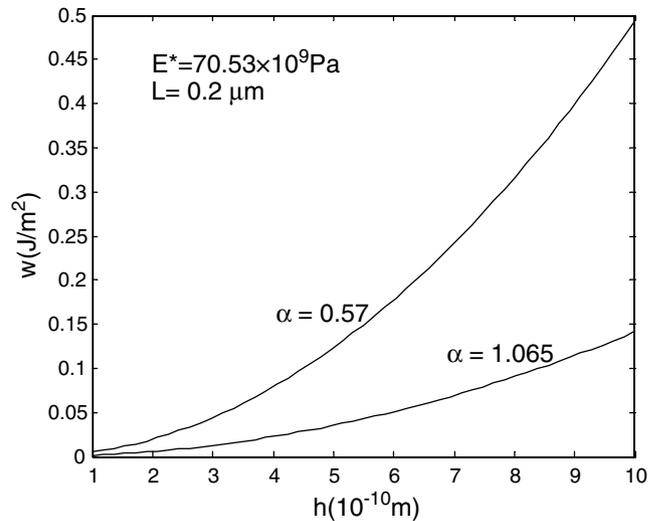

Fig. 4. Correlation of gap height h with wafer surface energies for $\alpha = 0.57$ and $\alpha = 1.065$.

Fig. 3. Correlation of gap height h with gap length L of wafer roughness for different values of α.
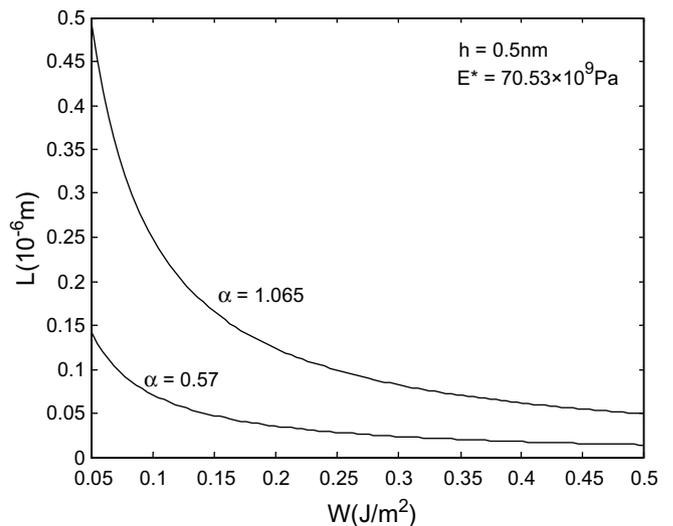

Fig. 5. Correlation of gap length L with wafer surface energies for $\alpha = 0.57$ and $\alpha = 1.065$.

Table 1
Experimental results of wafer direct bonding under different surface nano-scale roughness

Wafer pairs	L (µm)	h (nm)	Experimental results	α	Results of our model
A	0.147–0.182	1.2	Not bondable	0.342–0.381	Regime I
B	0.242–0.351	0.6	Spontaneous Bond with voids	0.878–1.058	Regime II
C	0.237–0.349	0.13	Self-propagating	4.014–4.871	Regime III
1[7]	0.301–0.472	1.2	With pressure, slow bond speed	0.49–0.614	Regime I&II
2[7]	0.329–0.493	1.1	With pressure, slow bond speed	0.559–0.684	Regime I & II
3[7]	0.125–0.166	1.0	Bonding with voids	0.379–0.437	Regime I
4[7]	0.114–0.174	0.9	Bonding with voids	0.402–0.497	Regime I
5[7]	0.20–0.378	<0.1	Self-propagating	4.794–6.59	Regime III

would be presented in another work since we focused on the effect of wafer roughness in this work. Because our model was based on a sinusoidal distribution for surface roughness, parameters of h and L can be estimated with the surface measurements of atom force microscopy. The experimental results were presented in Table 1 for wafer pairs A, B and C. The results showed that wafer pair A with large surface roughness, whose value of parameter α is estimated less than 0.381, bonding can not occur even with large external pressure, while wafer pair B with α between 0.878 and 1.058 can be bonded without external pressure, however, interfacial voids were observed under Infred camera. For wafer pair C with α between 4.014 and 4.871, no void was observed after spontaneous bonding.

Taking the experimental data from literature [7] for further verification, 5 bonding pairs with different surface roughness were considered, where parameters of h and L were estimated with experimental data, and the value α were calculated and shown in Table 1.The results showed that wafer pairs 1 and 2 bonded slowly after being brought into contact with external pressure, and a few voids were detected by means of the IR camera. Wafer pairs 3 and 4 were not bondable at all, even under pressure. Wafer pair 5 bonded spontaneously without any eternal pressure. The phenomenon was in reasonable agreement with analysis of our model. For wafer pairs 1 and 2, the value of parameter α remain in the interval which included the critical value 0.57, in other words, the surface roughness characteristics covered both regime I and II at the same time. According to the predictions of our model, one part of wafer surface would be able to bond with the application of pressure, and the other would bond with voids. For wafer pairs 3 and 4, because α was less than the critical value 0.57, the surface roughness parameters were in regime I, wafer would not bond at all even under the external force. For wafer pairs 5, because α was larger than the critical value 1.065, which was covered in regime III, the wafer pair could be bond spontaneously.

4. Conclusions

High surface waviness and roughness of wafers will result in failing to bond or bond with the formation of voids at the bonded interface. We propose a quantitative model to describe the sponta-neous bondability of wafers. Based on the model, a dimensionless analysis was carried out in detail for silicon wafer direct bonding under low temperature. The requirements of bonding surfaces and results of bonding can be predicted in a quantitative and non-destructive way through correlation of the surface energy and nano-topography of wafers. Based on the dimensionless analysis, and taking the dimensionless number α as a measure, three regions of silicon wafer bonding possibilities can be identified. When $\alpha < 0.57$ as in regime I, the wafer would not bond fully even with external force. When $0.57 < \alpha < 1.065$ as in regime II, the wafer can bond spontaneously with voids, when $\alpha > 1.065$ as in the regime III, the wafer would bond spontaneously with full contact or no voids.

Acknowledgements

References

[1] Q. Tong, U. Gösele, Semiconductor Wafer Bonding: Science and Technology, John Wiley & Sons, New York, 1999.
[2] U. Gösele, H. Stenzel, T. Martini, Appl. Phys. Lett 67 (1995) 3614.
[3] K.L. Johnson, K. Kendall, A.D. Roberts, Proc. Roy. Soc. Lon. Ser. A 324 (1971) 301.
[4] S. Farrens, J. Dekker, in: Proceedings of the Third International Symposium on Semiconductor Wafer Bonding: Physics and Applications, Reno, NV, 1995, p. 184.
[5] S. Bengtsson, K. Ljungberg, J. Vedde, Appl. Phys. Lett. 69 (1996) 3381.
[6] H. Yu, Z. Suo, J. Mech. Phys. Solids 46 (1998) 829.
[7] C. Gui, M. Elwenspoek, N. Tas, J. Appl. Phys 85 (1999) 7448.
[8] T. Martini, E. Schmidt, S. Mack, M. Reiche, H. Stenzel, S. Li, U. Gosele, Q. Tong, in: Proceedings of Third International Symposium on Semiconductor Wafer Bonding: Physics and Applications, Reno, NV, 1995, p. 147.
[9] M. Reiche, K. Scheerschmidt, D. Conrad, R. Scholz, A. Plossl, U. Gosele, K. Tu, Proc. Roy. Microsc. Soc. Conf. (1997) 447.
[10] D. Maugis, J. Colloid Interf. Sci. 150 (1992) 243.
[11] J.A. Greenwood, K.L. Johnson, E. Matsubara, Wear 100 (1984) 47.
[12] C.Y. Hui, Y.Y. Lin, J.M. Naney, E.J. Kramer, J. Polym. Sci. Part B: Polym. Phys. 39 (2001) 1195.