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Effect of surface characteristic on room-temperature silicon direct bonding

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ABSTRACT

Silicon direct bonding plays an important role in micro/nano-fabrication and integration. However, silicon surface when not in good condition will result in voids or gaps in the bonding interface or even a complete failure to bond. In this paper the effect of surface characteristic on room-temperature silicon direct bonding is investigated. It is found that the occurrence of bonding is related to surface energy, micro/nano-topography and elasticity of silicon wafers. Then a dimensionless parameter, α, is presented in detail, and two critical values, 0.570 and 1.065 are obtained: when $\alpha > 1.065$, indicating that the normalized combined force of both adhesion force and external force $\hat{F} \leq 0$ and $d\hat{F}/dc \leq 0$, the bonding wave will spread quickly and spontaneous bonding will occur; when $1.065 > \alpha > 0.57$, $\hat{F} \leq 0$ and it will facilitate silicon direct bonding but not guaranteeing bonding spontaneously; when $\alpha < 0.57$, $\hat{F} > 0$, the bonding resistance needs to be overcome for silicon bonding. If α is very close to 0.57 and enough external pressure is provided, silicon wafer pairs will bond slowly and voids or gaps may exist in the interface, otherwise they will fail to bond. Experiments of silicon direct bonding with wafers in different surface characteristics were used to verify the model. The analysis results prove that the model describes the experiments very well. Thus, the model provides a general route for assessing the impact of surface characteristic in direct bonding, and can be employed when evaluating different processes for silicon direct bonding applications.

1. Introduction

Silicon direct bonding (SDB), a flexible process in semiconductor manufacturing, allows one to join mirror-polished silicon wafers without the addition of any glue. Now it has been widely used in a range of applications, including the fabrication of silicon-on-insulator substrates, microelectronic devices, power electronic devices, micromechanic devices, optoelectronic devices, and three-dimensional microelectromechanical systems [1–4]. Nevertheless, it appears that most researchers and engineers, when considering the use of SDB at room temperature, are initially confronted with a number of down-to-earth questions and problems, and the bonding mechanism remains poorly understood. It is known that SDB has been attributed to the short-range intermolecular and interatomic attraction forces, such as Van der Waals forces [5]. Consequently, the silicon surface energy and topography become the most critical parameters in the process [6–8]. According to spatial frequency range, silicon surface topography is divided into global flatness, surface waviness and surface roughness. Commercially available prime grade silicon wafers of the usual thickness exhibit a global flatness variation of 1–3 μm. Variation of that order can easily be accommodated through mutual deformation of the wafers. Even a bow of up to 25 μm poses no serious obstacle to wafer bonding [4]. Thus, only surface waviness and roughness are concerned in this work. Certainly, silicon wafers with obvious surface waviness and roughness will result in a small area of contact, thus yield voids or gaps in the bonding interface even failing to bond [9].

The first theory on the problem of closing gaps between contacted wafers was proposed by Stengl et al. [10]. This gap-closing theory then was further developed by Tong and Gösele [5,11,12], and used to study the energy balance between the released energy during bonding and the energy increase due to the elastic distortion of the wafer. A detailed analysis of the three-dimensional elastic field in the misfit between contacted wafers has been presented by Yu and Hu [13], leading to the same results as the gap-closing theory. Spontaneous SDB, described as a special phenomenon particularly for hydrophilic silicon wafer bonding, in which the bonding wave can spread over the entire wafer surface smoothly, has also been discussed in the literature [14–17]. However, the mechanism of spontaneous wafer bonding has not been revealed yet, and no accurate quantitative model for this process exists to date. In the present study, the silicon surface characteristic in room-temperature SDB is modeled based on the Johnson–Kendall–Roberts (JKR) theory [18]. Experiments are carried out and analyzed to verify the model.

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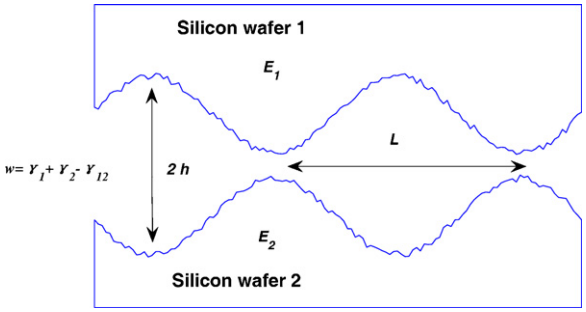

Fig. 1. Cross-section of two silicon wafers in contact for direct bonding.

2. Dimensional analysis

As depicted in Fig. 1, there are basically three factors relevant to the SDB process [19]: the material deformability, commonly expressed as its Young's modulus E [N m^{-2}]; the specific surface energy of adhesion, w [N m^{-1}]; and the surface roughness of both wafers. In order to simplify the problem, the surface roughness are characterized by two variables: length L [m] and height h [m] of the gap between two wafers. Besides, the thickness of wafers also plays an important role in the bonding. Christiansen et al. investigated the bondability of wafers in different thickness conditions [4]. Turner et al. found that bonding difficulty increased with the cube of thickness [6]. Here in this work we only focus on the effect of surface characteristic on room-temperature SDB. It is clear that bonding will be easier if the surface energy of adhesion is large (w big) and the material is readily deformable (E small). So the criterion may have something to do with the ratio w/E, which has the dimension of length [m]. On the other hand, if the silicon surfaces are smooth enough (h small) and have large wavelengths L, it is also easier for wafer bonding as they do not need to be deformed much. Therefore, a criterion for bondability with a simplest dimensionless combination of w, E, h and L gives a sensible result

$$\propto \left(\frac{w}{E}\cdot\frac{L}{h^2}\right)^c \tag{1}$$

where c is a constant.

3. Surface characteristic modeling for room-temperature SDB

It was agreed that the JKR theory is valid for solids with a large surface energy [20]. This is generally the case for hydrophilic SDB, because the silicon wafer surface roughness is in the range of micro/nano-scale where the adhesion forces between contact wafers are dominant. To evaluate the effect of surface characteristic on silicon direct bonding, a model considering the surface geometry is required. Yu and Suo presented a model in the context of direct bonding in which there is a sinusoidal varying gap at the interface, and the gap must be closed through elastic deformation during bonding [13]. Here we consider a similar way to explore the problem. In our model the asperities of silicon wafers are assumed to be periodically distributed instead of a random distribution, where the gap between silicon wafers are caused by a flatness nonuniformity with a lateral periodic extension L much larger than the gap height, h_1 and h_2, as schematically shown in Fig. 2(a).

According to Greenwood's conclusions [21], the effect of a model considered roughness on two surfaces with the original height distribution h_i is equivalent to the model assumed that one of the contact surfaces (the lower silicon wafer) is perfectly rigid flat not deforming in the contact, and the other (the upper silicon wafer) has a combined height distribution h, as shown in Fig. 2(b). Here the solid lines indicate the silicon wafers contact interfaces before bonding, and the dashed lines indicate the interfaces in the bonding. We need to emphasize that the combined height h in the model in Fig. 2(b) is not measurable. We can only measure the original height h_i in Fig. 2(a) from the experiment, and then try to get the equivalent combined height h. This was not considered in the literature [14], thus, the available experimental data could not verify their theory reasonably.

The cross-sectional surface micro/nano-profile of the upper silicon wafer in the equivalent model in Fig. 2(b) is considered as a periodically nonnegative special case examined by Johnson [22]

$$f(x) = \frac{L^2}{2R\pi^2}\ \sin^2\left(\frac{\pi x}{L}\right), \qquad x\in(kL-x_0, kL+x_0), \quad 2x_0 \le L \tag{2}$$

where k is an integer, x_0 is the length of contacted zones, R is the mean cap radius, and L is the periodic length of the gap. Here the combined maximum height of the gaps is given by

$$h = \frac{L^2}{2R\pi^2} \tag{3}$$

Note that for small x

$$f(x) \approx \frac{x^2}{2R}$$

which is the usual Hertzian approximation for a cylinder of radius R. According to the contact mechanics of surfaces of periodic roughness, the pressure distribution underneath the asperities inside the contacted zones can be deduced [23]

$$p(x) = \frac{\cos(\pi x/L)}{\sqrt{\sin^2(\pi x_0/L) - \sin^2(\pi x/L)}} \times \left\{\frac{E^* L}{4\pi R}\left[\sin^2\left(\frac{\pi x_0}{L}\right) - 2\sin^2\left(\frac{\pi x}{L}\right)\right] + \frac{F}{L}\right\} \tag{4}$$

where F is the force per asperity on the wafer surface, contributed by both the adhesion force and the external force, and E^* is the

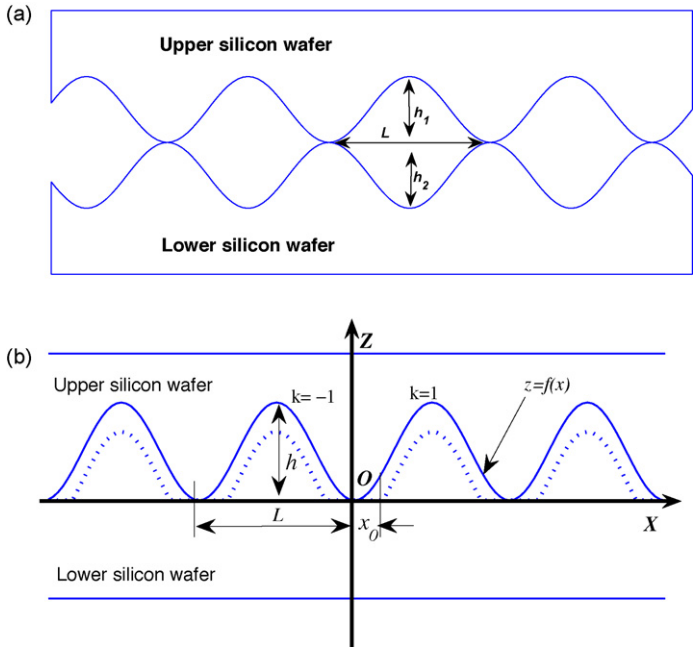

Fig. 2. The schematic model for SDB with periodically distributed asperities. (a) The model considered roughness on two surfaces with measurable height distribution h_i; (b) the equivalent model with one perfectly rigid flat not deforming in the contact and the other having a combined height distribution h, where the solid lines indicate the silicon wafers contact interfaces before bonding, and the dashed line the interfaces in the bonding.