



A MODEL OF WAFER BONDING BY ELASTIC ACCOMMODATION

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ABSTRACT

Two clean and flat wafers can adhere spontaneously. The technique has recently led to novel electronic and optoelectronic devices. The adhesion arises from short-range interatomic forces between wafer surfaces, which can be represented by a reduction in surface energy associated with the transformation of two surfaces into one interface. The wafers, however, are seldom perfectly flat; the misfit has to be accommodated by elastic distortion, plastic deformation, or mass transport. We model elastic accommodation in this paper. The distortion causes the wafers to gain elastic energy. If the surface reduction dominates over the elastic energy gain, the wafers will bond. We solve the three dimensional elastic field in the misfit wafers analytically. The conditions for bonding are established, and practical implications discussed. © 1998 Elsevier Science Ltd. All rights reserved

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INTRODUCTION

Glass surfaces can be polished so flat that, when meticulously cleaned, they can adhere under a slight pressure at room temperature. The joint hardly reflects light, and is suitable for making optical instruments. The ability to form such an “optical contact” is not unique to glasses: Obreimoff (1930) showed that two freshly split mica sheets could adhere again. Rayleigh (1936) noted that, although contacted glasses could not be slid over one another by any force which was possible to apply by fingers, they could be wedged apart readily. He found that the work needed to separate the contact was much lower than that to break the bulk glass. The effect of heat treatment has also long been appreciated. Parker and Dalladay (1917) demonstrated that contacted glasses, heated for some time, would unite to a single piece, which could not be separated without breaking the glasses themselves. The temperature at which the union takes place must be kept sufficiently low, so that the pieces are hard enough to withstand clamping and handling.

The technique has recently been developed to bond semiconductor wafers, leading to electronic and optoelectronic devices of much superior performance; see Haisma *et al.* (1994) Babic *et al.* (1995), and Liao (1997) for lists of example. The main advantage of the technique is that it can integrate dissimilar materials while retain

their crystalline perfection—that is, if one or both wafers are perfect crystals before contact, the perfection is retained after bonding, except for a few atomic layers at the interface. For example, after InP and GaAs wafers are bonded, cube on cube in crystalline orientation, arrays of dislocations form on the interface to offset the difference in lattice constants, but no dislocations are added to the bulk of either wafer (e.g., Wada *et al.*, 1993). By contrast, a layer of InP grown on a GaAs substrate would contain a large number of dislocations inside the InP crystal.

The basic cause for bonding is the attractive interatomic force between two surface. Being short ranged, the force acts like a zip: the adhesion starts from one point of initial contact, and spreads over a macroscopic area. The effect of the force can be represented by surface energies. Let γ_1 and γ_2 be the surface tensions of the two wafers before bonding, and γ_{12} be the interface tension after bonding. Provided the sum of the two surface tensions exceeds the interface tension, $\gamma_1 + \gamma_2 > \gamma_{12}$, when the two surface unite to form the interface, the net free energy reduces. It is this reduction, known as the Dupré work of adhesion

$$\Gamma = \gamma_1 + \gamma_2 - \gamma_{12}, \quad (1)$$

that motivates bonding. The necessary condition for the two wafers to adhere, $\Gamma > 0$, can often be satisfied after surface treatment.

Yet in everyday experience solids seldom stick spontaneously. The main reason is that two solid surfaces never match perfectly. At the atomic scale, the two solids meet at a few points, holding other atoms too far apart to interact. The surfaces can, however, become matching by mass diffusion or viscous flow. At an elevated temperature, motivated by the work of adhesion, atoms move from contact points into gaps. The process is the same as in sintering ceramic or glass powders. At a low temperature, when mass transport is too slow, plastic deformation can match two wafers, provided at least one of the mating solids is plastically deformable and a large pressure is applied. Suga *et al.* (1992), for example, have pressed metals and ceramics into adhesion.

The above procedures to remove surface asperity have limitations. When two wafers have a large difference in thermal expansion coefficients, heat treatment would induce high residual stresses upon cooling, which may crack the wafers. Heat treatment may also destroy dopant profile in semiconductors; for example, Wada and Kamijoh (1994) observed that a high temperature treatment would degrade photoluminescence of a Si–InP joint. When both wafers are brittle, as semiconductors are, plastic accommodation is impossible. On such occasions, one has to join wafers without the aid of intense heat or large force. Indeed, Gösele *et al.* (1995) demonstrated that two flat silicon wafers, cleaned in vacuum, could form covalent bonds.

For wafers to bond at the room temperature, in the absence of large external pressure, the misfit gap between the wafers must be accommodated by elastic distortion. Figure 1 illustrates the problem. Prior to contact two wafers are not perfectly flat (Fig. 1(a)). Once brought together, they contact at a few points first (Fig. 1(b)). In this state, the total free surface area is large, and so is the free energy. To reduce the free energy, the wafers deform elastically and transform the free surfaces into an interface. If the misfit is large, the wafers gain too much elastic energy, and will bond only over patches of the surface area, leaving the rest of the area unbonded (Fig.

1(c)). If the misfit is small, the wafers gain a small amount of elastic energy, and will bond over the entire area (Fig. 1(d)). This paper analyzes the elastic field in the misfit wafers, and establishes bonding conditions.

THE MODEL

Some early works are related. Rayleigh (1936) studied the contact between a lens and a flat plate. After meeting at one point, they both distort locally to allow the

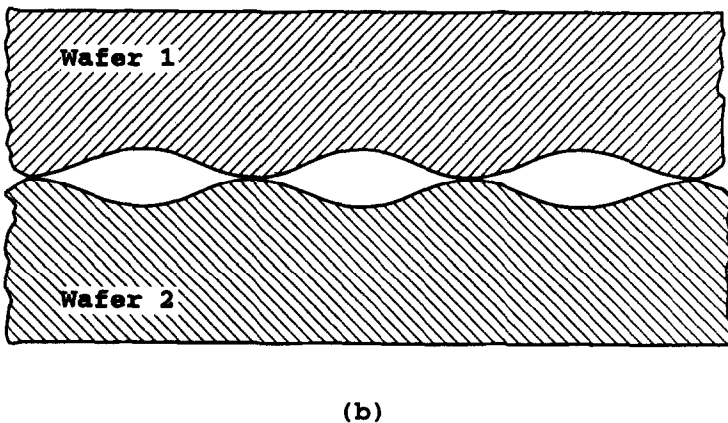
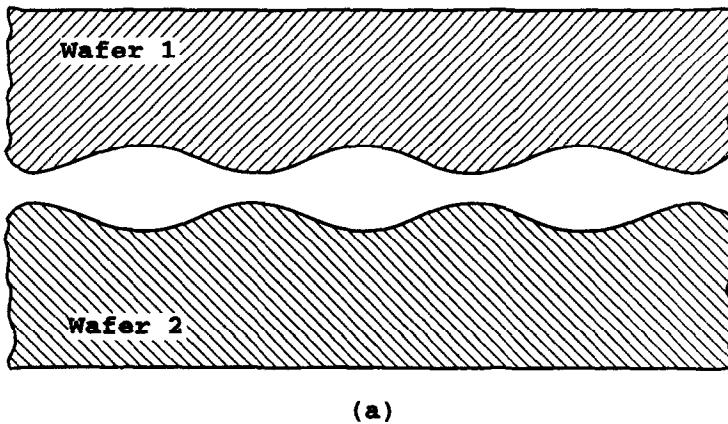
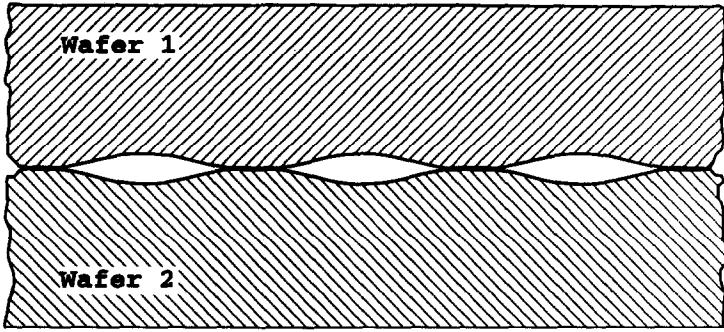
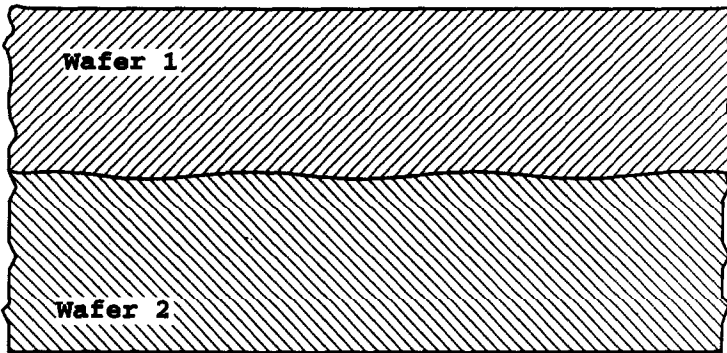


Fig. 1. (a) Before contact, the two wafer surfaces do not match. (b) When placed in contact, the wafers first meet at points. (c) Under the action of adhesive force, the wafers deform to spread the bond over patches of the area. (d) If the magnitude of the gap is small, the adhesive force can close the gap completely.

Residual stress field is induced in both (c) and (d).



(c)



(d)

Fig. 1—Continued.

bond to spread over an area. The bonded area is large if the lens has a large radius of curvature. Johnson *et al.* (1971) modeled this phenomenon by adding adhesion to the Hertz theory of contact between smooth elastic bodies. The model predicted a contact area under no external force, and a force needed to separate the bodies; both were observed experimentally. They used large rubber and gelatine spheres in the experiment to obtain large adhesion areas. Nix (1997) modeled surface joining as an origin of stress in thin films due to island coalescence. Maszara *et al.* (1991) detected a periodic strain field near the interface of a bonded pair of silicon wafers by using X-ray topography. They also scanned the free surfaces by using an optical profilometer, and performed a spectrum analysis to obtain the amplitude of roughness as a function of wavelength. The wavelength of the strain field in the bonded wafers was found to

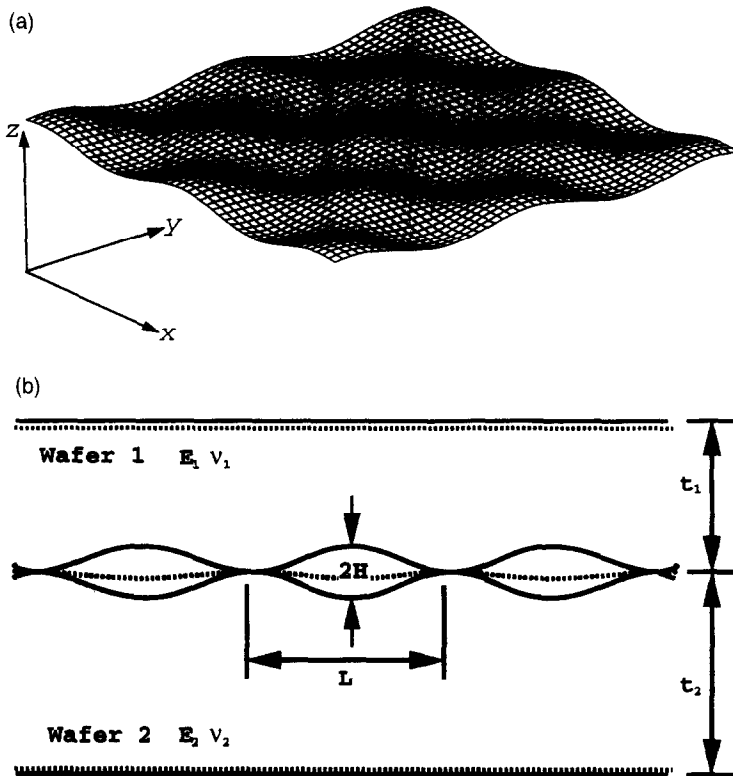


Fig. 2. (a) The misfit gap varies sinusoidally in the plane of the interface. (b) The geometry of a cross section normal to the interface.

be comparable to that of the dominant component of the free surface roughness. Tong and Gösele (1994, 1995) considered the effect of elasticity on wafer bonding. They gave expressions of bonding conditions in the limits of very thin and very thick wafers.

In this paper, we will analyze the model of Tong and Gösele (1994, 1995) in full ranges of parameters. To the best of our knowledge, such a comprehensive analysis has not been done before. With reference to Fig. 2(a), the interface is nominally perpendicular to the z direction, and the misfit gap is taken to be sinusoidal in both the x and y directions. Figure 2(b) sketches a cross section of the joint, where for clarity the ratio H/L has been greatly exaggerated. The solid curves represent the surfaces before bonding, with the sinusoidal gap of wavelength L and amplitude $2H$. The dashed curve represents the interface after bonding. The upper wafer, wafer 1, has Young's Modulus E_1 , Poisson's ratio ν_1 , and thickness t_1 . The corresponding values for the lower wafer are E_2 , ν_2 , and t_2 .

We assume that the wafers will bond over the entire area if the elastic energy gained in closing the gap is less than the surface energy reduction. The following dimensional considerations reveal several main features of the problem. For simplicity we consider

here the case where the misfit wavelength is much smaller than the thickness of either wafer, $L \ll t_1$ and $L \ll t_2$. Consider one period of the bonded wafers, namely, a column of material normal to the interface, of a square cross-sectional area L^2 . After bonding, the misfit induces an elastic strain field of magnitude scaled as H/L ; the larger the gap height and the smaller the wavelength, the larger the strain. The elastic energy per unit volume scales as $E^*(H/L)^2$, where E^* is an appropriate elastic modulus. Under the assumptions that $L \ll t_1$ and $L \ll t_2$, the stress field is localized near the interface, and decays in the z direction beyond the length scale L . Consequently, the elastic energy per period of the bonded wafers, U , scales as

$$U \propto E^*(H/L)^2 L^3.$$

The surface energy reduction per period of the joint is ΓL^2 . The dimensionless ratio of the two energies is

$$\eta = \frac{E^* H^2}{\Gamma L}. \quad (2)$$

When the ratio is below a critical value, denoted as η_c , the wafers will bond over the entire area. When the ratio is above the critical value, the wafers will bond over patches of the area. The analysis in a later section will show that $\eta_c = 3.60$ for thick wafers. That is, two wafers will bond over the entire area if

$$\frac{E^* H^2}{\Gamma L} < 3.60.$$

Taking representative values, $\Gamma = 1 \text{ N/m}$ and $E^* = 10^{11} \text{ N/m}^2$, one concludes from eqn (2) that, for example, when $L = 10 \text{ } \mu\text{m}$, $2H_c = 38 \text{ nm}$ is the largest gap height that can be accommodated by elasticity. When $L = 1 \text{ mm}$, $2H_c = 380 \text{ nm}$. Complete bonding is more likely for wafers with low elastic moduli, small misfit height, large misfit wavelength, and large Dupré work of adhesion. Also note that the absolute length scale of the misfit is important: for two geometrically similar gaps (i.e., having an identical ratio H/L), the gap with a smaller length scale is more likely to bond completely.

In the following three sections, we will first describe an elasticity analysis of a pair of misfit wafers, then apply the results to establish conditions for wafer bonding, followed by a discussion of practical aspects of wafer bonding related to the model.

ELASTIC FIELD IN MISFIT WAFERS

The ratio H/L is taken to be so small that the linear elasticity theory applies. Let $(u_1, u_2, u_3) = (u, v, w)$ be the displacement field, which obeys Navier's equation:

$$(1 - 2\nu)u_{i,jj} + u_{i,jj} = 0. \quad (3)$$

The stresses, σ_{ij} , relate to the displacements as

$$\sigma_{ij} = \frac{E}{1+\nu} \left[\frac{1}{2}(u_{i,j} + u_{j,i}) + \frac{\nu}{1-2\nu} u_{k,k} \delta_{ij} \right]. \quad (4)$$

In the above, $\delta_{ij} = 1$ when $i = j$, and $\delta_{ij} = 0$ when $i \neq j$. The elastic constants E and ν take different values in two wafers.

The following procedure was used in another context by Yang and Suo (1995). To accommodate the sinusoidal gap, the displacement field is expected to take the form

$$\begin{aligned} u &= \sin(kx) \cos(ky) f(kz) \\ v &= \cos(kx) \sin(ky) f(kz) \\ w &= w_0 + \cos(kx) \cos(ky) g(kz) \end{aligned} \quad (5)$$

where $k = 2\pi/L$, and w_0 represents a rigid body translation. The functions f and g are determined by substituting eqn (5) and eqn (3), giving

$$\begin{aligned} (1-2\nu)f''' - 4(1-\nu)f - g' &= 0 \\ (1-\nu)g'' - (1-2\nu)g + f' &= 0 \end{aligned} \quad (6)$$

with $(\cdot)' = d(\cdot)/d(kz)$. These are ordinary differential equations of constant coefficients, to which the solution is

$$\begin{aligned} f(kz) &= [a_1 + a_2 kz] e^{\sqrt{2}kz} + [a_3 + a_4 kz] e^{-\sqrt{2}kz} \\ g(kz) &= [-\sqrt{2}a_1 + (3-4\nu-\sqrt{2}kz)a_2] e^{\sqrt{2}kz} + [\sqrt{2}a_3 + (3-4\nu+\sqrt{2}kz)a_4] e^{-\sqrt{2}kz}. \end{aligned} \quad (7)$$

The coefficients a_i are to be determined by boundary conditions.

We next apply solution (7) to wafer 1 under the following boundary conditions: (i) on the free surface ($z = t_1$) the normal stress vanishes, (ii) on the free surface ($z = t_1$) the shear stress vanishes, (iii) on the interface ($z = 0$) the shear stress vanishes, and (iv) on the interface ($z = 0$) the vertical displacement is

$$w_1 = -\frac{H_1}{2} [1 + \cos(kx) \cos(ky)]. \quad (8)$$

The constant H_1 is the amplitude of the normal surface displacement of wafer 1. The four boundary conditions determine the four coefficients, giving

$$\begin{aligned} a_1 &= -\frac{H_1}{4(1-\nu_1)} \frac{-4(kt_1)^2 + (1-2\nu_1)(2\sqrt{2}kt_1 - e^{-\sqrt{2}2kt_1} + 1)}{\sqrt{2}(e^{2\sqrt{2}kt_1} - e^{-2\sqrt{2}kt_1} + 4\sqrt{2}kt_1)} \\ a_2 &= -\frac{H_1}{4(1-\nu_1)} \frac{2\sqrt{2}kt_1 - e^{-\sqrt{2}2kt_1} + 1}{e^{2\sqrt{2}kt_1} - e^{-2\sqrt{2}kt_1} + 4\sqrt{2}kt_1} \\ a_3 &= \frac{H_1}{4(1-\nu_1)} \frac{4(kt_1)^2 + (1-2\nu_1)(2\sqrt{2}kt_1 + e^{\sqrt{2}2kt_1} - 1)}{\sqrt{2}(e^{2\sqrt{2}kt_1} - e^{-2\sqrt{2}kt_1} + 4\sqrt{2}kt_1)} \\ a_4 &= -\frac{H_1}{4(1-\nu_1)} \frac{2\sqrt{2}kt_1 + e^{\sqrt{2}2kt_1} - 1}{e^{2\sqrt{2}kt_1} - e^{-2\sqrt{2}kt_1} + 4\sqrt{2}kt_1}. \end{aligned} \quad (9)$$

Once these coefficient are determined, all components of the displacements and stress fields are determined in wafer 1. In particular, the stress component $(\sigma_{zz})_1$ is

$$(\sigma_{zz})_1 = \frac{\bar{E}_1 k H_1 \cos(kx) \cos(ky)}{2\sqrt{2}(e^{2\sqrt{2}kt_1} - e^{-2\sqrt{2}kt_1} + 4\sqrt{2}kt_1)} \times \begin{bmatrix} (-4(k t_1)^2 - 2\sqrt{2}kt_1 + e^{-2\sqrt{2}kt_1} - 1)e^{\sqrt{2}kz} \\ + (2\sqrt{2}kt_1 - e^{-2\sqrt{2}kt_1} + 1)(\sqrt{2}kz)e^{\sqrt{2}kz} \\ + (-4(k t_1)^2 + 2\sqrt{2}kt_1 + e^{2\sqrt{2}kt_1} - 1)e^{-\sqrt{2}kz} \\ + (2\sqrt{2}kt_1 + e^{2\sqrt{2}kt_1} - 1)(\sqrt{2}kz)e^{-\sqrt{2}kz} \end{bmatrix} \quad (10)$$

with

$$\bar{E}_1 = \frac{E_1}{1 - \nu_1^2}. \quad (11)$$

On the interface ($z = 0$), the stress is

$$(\sigma_{zz})_1 = \frac{\bar{E}_1 k H_1}{2\sqrt{2}} I(kt_1) \cos(kx) \cos(ky), \quad (12)$$

where

$$I(a) = \frac{e^{2\sqrt{2}a} + e^{-2\sqrt{2}a} - 2 - 8a^2}{e^{2\sqrt{2}a} - e^{-2\sqrt{2}a} + 4\sqrt{2}a}. \quad (13)$$

We can apply the same procedure to wafer 2. Take the vertical displacement of wafer 2 to be

$$w_2 = + \frac{H_2}{2} [1 + \cos(kx) \cos(ky)]. \quad (14)$$

Similar expressions can be obtained by proper substitutions in the above. Specifically, on the interface $z = 0$, the normal stress component in wafer 2 is

$$(\sigma_{zz})_2 = \frac{\bar{E}_2 k H_2}{2\sqrt{2}} I(kt_2) \cos(kx) \cos(ky). \quad (15)$$

We next determine the two amplitudes, H_1 and H_2 . After bonding, the normal displacement of the surface of wafer 2 relative to that of wafer 1 is

$$w_2 - w_1 = H[1 + \cos(kx) \cos(ky)]. \quad (16)$$

The is, the amplitude of the relative displacement should equal that of the misfit gap, $H_1 + H_2 = 2H$. Equilibrium requires that the normal stress on the interface be continuous, $(\sigma_{zz})_1 = (\sigma_{zz})_2$. These two conditions give

$$H_1 = \frac{2H\bar{E}_2 I(kt_2)}{\bar{E}_1 I(kt_1) + \bar{E}_2 I(kt_2)}, \quad H_2 = \frac{2H\bar{E}_1 I(kt_1)}{\bar{E}_1 I(kt_1) + \bar{E}_2 I(kt_2)}. \quad (17)$$

Now the displacements and stresses are directly related to the misfit gap amplitude, H .

To appreciate the distribution and magnitude of the stress field, we now examine in some detail the stress component σ_{zz} . The general expression in wafer 1 is given by eqn (10), where H_1 should be replaced by that in eqn (17). The normal stress at the interface is

$$\sigma_{zz} = \frac{kH}{\sqrt{2}} \cos(kx) \cos(ky) \left(\frac{1}{\bar{E}_1 I(kt_1)} + \frac{1}{\bar{E}_2 I(kt_2)} \right)^{-1}. \quad (18)$$

This expression will be used in the next section to establish the critical bonding condition.

Next consider the limiting case where both wafers are so thick that $L \ll t_1$ and $L \ll t_2$, so that $I(kt_1) = I(kt_2) = 1$. Equation (10) is specialized to

$$(\sigma_{zz})_1 = \frac{kH\bar{E}_1\bar{E}_2}{\sqrt{2}(\bar{E}_1 + \bar{E}_2)} \cos(kx) \cos(ky) (1 + \sqrt{2}kz)e^{-\sqrt{2}kz}. \quad (19)$$

The stress varies periodically in the x and y directions, and decays exponentially in the z direction. The maximum occurs on the interface, its magnitude being

$$(\sigma_{zz})_{\max} = \frac{\sqrt{2}\pi H\bar{E}_1\bar{E}_2}{L(\bar{E}_1 + \bar{E}_2)}. \quad (20)$$

Taking the representative values $\bar{E}_1 = \bar{E}_2 = 10^{11} \text{ N/m}^2$, one finds the magnitude of the stress to be 222 MPa when $H/L = 10^{-3}$. The stress magnitude is linear in H/L . The dependence on elastic moduli is also clear. If the two wafers have a similar elastic modulus, the stress is proportional to the modulus. If one wafer is much stiffer than the other, the stress is essentially proportional to the modulus of the compliant wafer.

Figure 3 displays the stress magnitude, $(\sigma_{zz})_{\max}$ for wafers of intermediate thickness. Because of the symmetry, we need only consider cases where $t_1 \leq t_2$. The stress increases with the wafer thickness, and reaches plateau when the wafers are sufficiently thick, say, $t/L > 0.5$, corresponding to the limit eqn (20). Figures 3(b) and (c) show the effect of elastic moduli. When wafer 1 is less stiff than wafer 2, the thickness of wafer 2 has negligible effect on stress. When wafer 1 is stiffer than wafer 2, the thickness of wafer 2 can have appreciable effect on stress.

CRITICAL CONDITION FOR BONDING

The elastic energy stored in the two wafers after complete bonding can be computed by the work done by σ_{zz} at the interface to close the misfit gap. The elastic energy per period of the joint is

$$U = \frac{1}{2} \int_0^L \int_0^L (w_2 - w_1) \sigma_{zz} dx dy. \quad (21)$$

Using expressions (16) and (18), and integrating eqn (21), we obtain that

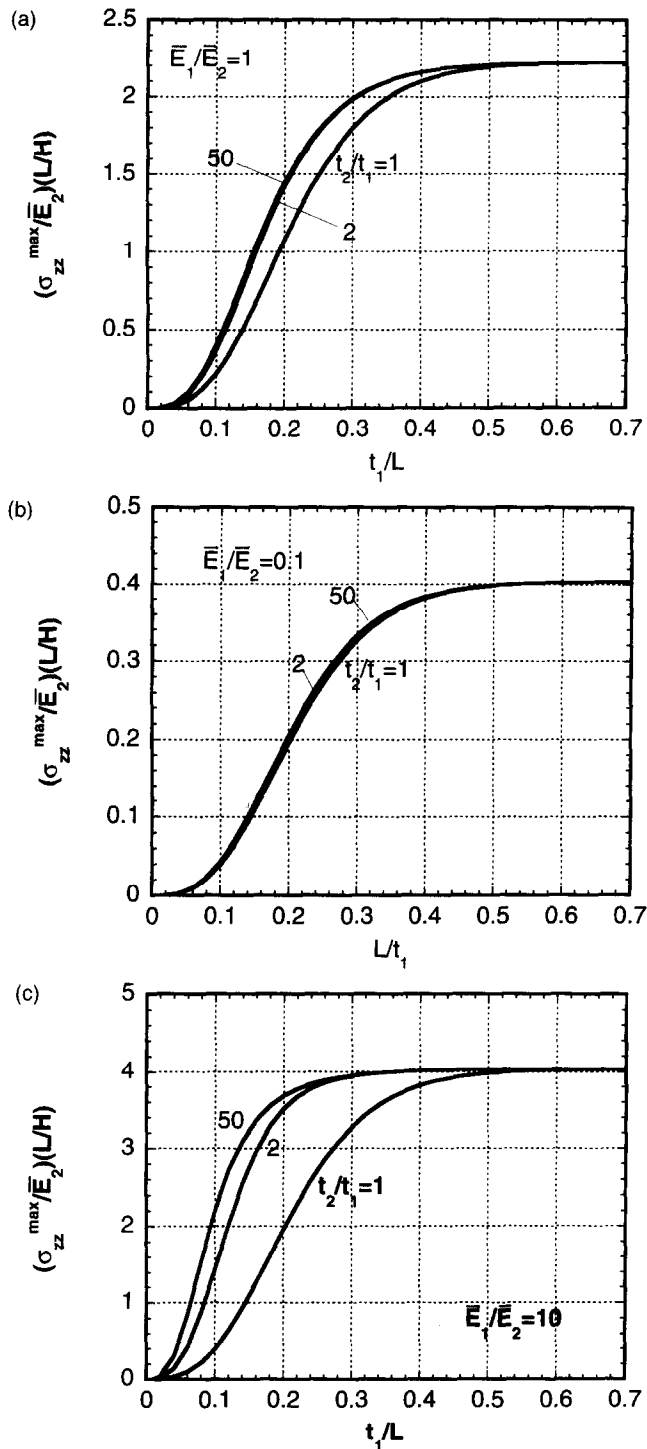


Fig. 3. Magnitude of the stress on the interface. (a) $\bar{E}_1/\bar{E}_2 = 1$, (b) $\bar{E}_1/\bar{E}_2 = 0.1$, (c) $\bar{E}_1/\bar{E}_2 = 10$.

$$U = \frac{\pi H^2 L}{4\sqrt{2}} \left(\frac{1}{\bar{E}_1 I(kt_1)} + \frac{1}{\bar{E}_2 I(kt_2)} \right)^{-1}. \quad (22)$$

When the two surfaces transform into one interface, the free energy per period of the joint changes by $U - \Gamma L^2$. Complete bonding occurs if this free energy change is negative, namely,

$$U - \Gamma L^2 < 0. \quad (23)$$

Replacing U with the expression (22), we find the critical condition for bonding:

$$\frac{H_c^2}{\Gamma L} = \frac{4\sqrt{2}}{\pi} \left(\frac{1}{\bar{E}_1 I(kt_1)} + \frac{1}{\bar{E}_2 I(kt_2)} \right). \quad (24)$$

Here $2H_c$ stands for the critical misfit amplitude. If the misfit amplitude is below this critical value, the two surfaces will bond over the entire area. If the misfit amplitude is above this critical value, the two surfaces will only bond over patches of the area. Note that the parameter grouping is equivalent to that anticipated in the Introduction.

The above condition looks complicated because of the function $I(x)$ defined in eqn (13). Two limits are helpful:

$$I(x) \rightarrow \begin{cases} \frac{\sqrt{2}}{3} x^3 & \text{as } x \rightarrow 0 \\ 1 & \text{as } x \rightarrow \infty \end{cases}. \quad (25)$$

We next use them to discuss the bonding criterion (24).

First consider the limit where the misfit wavelength is much smaller than the thickness of either wafer, $L \ll t_1$ and $L \ll t_2$, so that $I(kt_1) = I(kt_2) = 1$. Further assume that the elastic constants of the two wafers are identical. The bonding criterion (24) is simplified to

$$H_c = 1.90 \left(\frac{\Gamma L}{\bar{E}} \right)^{1/2}. \quad (26)$$

This result has the same form as that given by Tong and Gösele (1994, 1995), except for the coefficient. Because these authors did not give details of the model in their papers, we do not know the origin of the difference. Under the same assumptions, $L \ll t_1$ and $L \ll t_2$, if the elastic constants of the two wafers are different, eqn (24) becomes

$$H_c = 1.34 \left[\Gamma L \left(\frac{1}{\bar{E}_1} + \frac{1}{\bar{E}_2} \right) \right]^{1/2}. \quad (27)$$

When one wafer is much stiffer than the other, the misfit is mainly accommodated by the elasticity of the more compliant wafer, and the elastic constants of the stiffer wafer plays little role.

Next consider another limit where the two wafers are identical, and the thickness,

$t_1 = t_2 = t$, is much smaller than the misfit wavelength, $t \ll L$. The condition (24) is simplified to

$$H_c = 0.176 \sqrt{\frac{\Gamma L^4}{\bar{E} t^3}}. \quad (28)$$

The result is the same as that given by Tong and Gösele (1994, 1995), who derived it by using the thin plate theory.

Figure 4 displays the critical condition (24) for a range of parameters. Figure 4(a) plots the dimensionless ratio $\bar{E}_2 H_c^2 / \Gamma L$ as a function of the reduced misfit wavelength L/t_1 , for several values of t_2/t_1 , with $\bar{E}_1/\bar{E}_2 = 1$. Judging from the figure, it is evident that the short wavelength limit, eqn. (26), is a good approximation if, say, $L/t_1 < 2$. Everything else being equal, thinner wafers are easier to bond. Figure 4(b) plots the critical bonding conditions for the case where the thinner wafer is less stiff, $\bar{E}_1/\bar{E}_2 = 0.1$; the thickness of wafer 2 affect bonding negligibly. Figure 4(c) plots the corresponding results for the case where the thinner wafer is stiffer, $\bar{E}_1/\bar{E}_2 = 10$; the thickness of wafer 2 affects bonding significantly.

Yablonovitch *et al.* (1987) has developed a technique called epitaxial lift-off, where a very thin film is taken away from the substrate on which it is grown, and then bonded to another substrate. This flexible thin film can readily accommodate some nonflatness of the substrate. Figure 5 displays the critical conditions for the case where wafer 1 is much thinner than wafer 2, $t_1 \ll t_2$. The effect of elastic moduli is more readily seen in this graph.

DISCUSSION

Surface geometry aside, surface chemistry plays an important role. Foreign molecules usually adsorb on wafer surfaces, and lower the work of adhesion. Obreimoff (1930) observed that a smaller force could split mica in air than in vacuum. A large body of data now exists concerning the environmental effect on fracture energy (Lawn, 1993). An "optical contact" formed in the air at room temperature most likely arise from van der Waals or other weak bonds between the adsorbed molecules. Another role of heat treatment, aside from activating mass transport to match the surface geometry, is to activate reactions at the interface to convert the weak bonds into strong bonds. Stengl *et al.* (1989) discussed in some detail such interfacial reactions in silicon wafer bonding. At room temperature water molecules adsorbed on the surfaces form hydrogen bonds. At about 700°C, the water molecules diffuse away from the interface, and strong Si—O—Si bonds form. Using a double-cantilever-beam fracture specimen, Maszara *et al.* (1988) measured the work needed to separate a pair of silicon wafers (i.e., the work of fracture) as a function of annealing temperature. The work of fracture increases with the annealing temperature even when temperature is too low to activate viscous flow. The data clearly show the role of interfacial chemical changes on wafer bonding. The model discussed in the present paper does not specify the type of bonding, so long as the work of adhesion is positive.

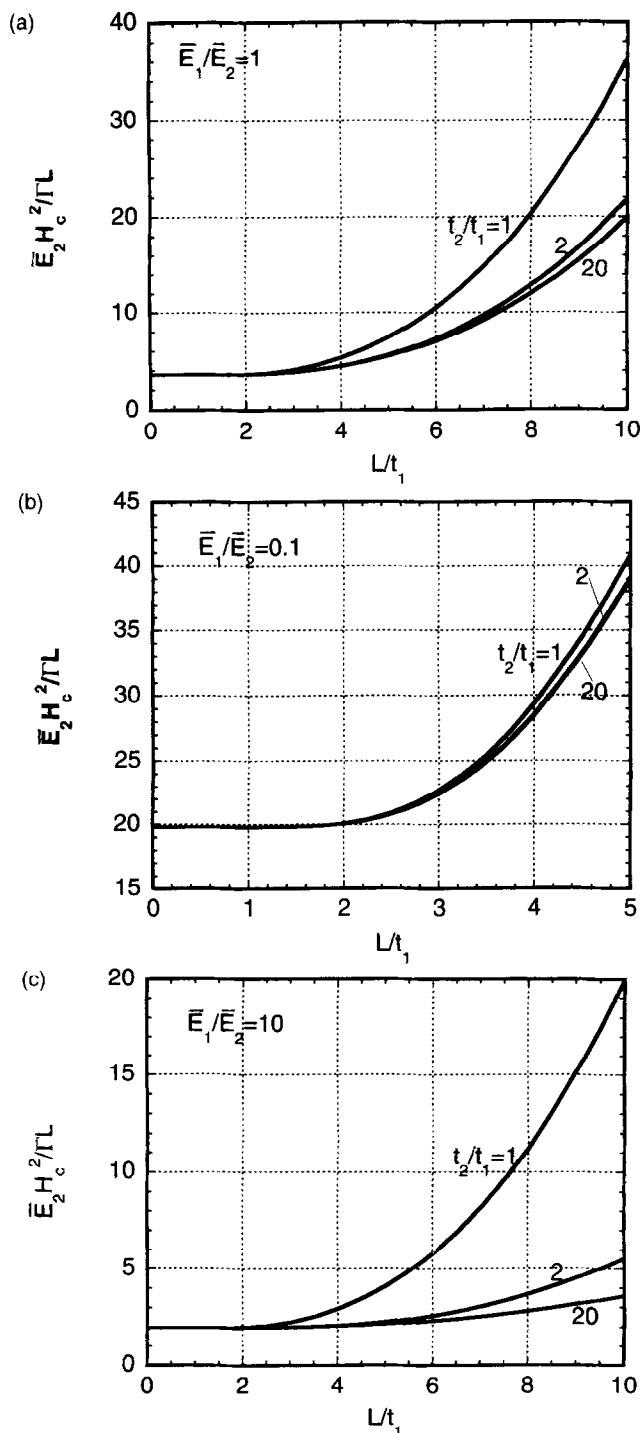


Fig. 4. The critical conditions for the wafers to bond over entire area. (a) $\bar{E}_1/\bar{E}_2 = 1$, (b) $\bar{E}_1/\bar{E}_2 = 0.1$, (c) $\bar{E}_1/\bar{E}_2 = 10$.

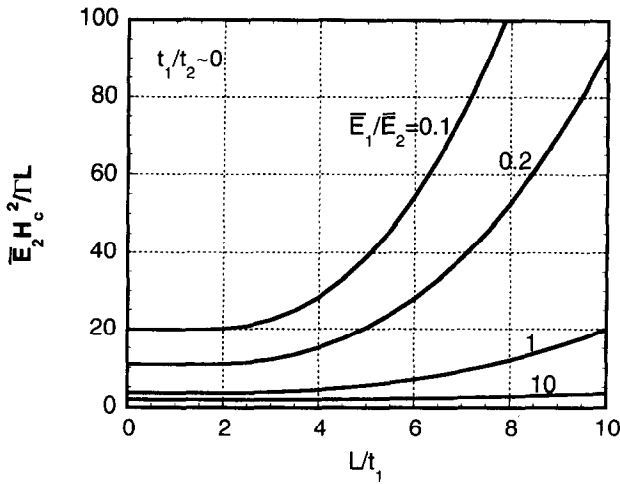


Fig. 5. The critical conditions for the case where one wafer is much thinner than the other, $t_1 \ll t_2$.

The effects of chemical changes enter the model through the value of the work of adhesion.

Two points are of practical significance. First, the temperature to activate the interfacial reactions may be much lower than that to activate mass transport to match the geometry. Thus, if before contact two wafers are polished so flat that elasticity will accommodate the misfit, one should expect that the wafers will attain a strong bond at a low temperature. Second, procedures may be applied to the wafers before contact to activate the surfaces, namely, remove molecules that prevent strong bonds. Examples include etching surfaces by an argon beam (Takagi *et al.*, 1996), exposing surfaces to a low power oxygen plasma (Farrens *et al.*, 1995), and placing wafers in ultrahigh vacuum (Gösele *et al.*, 1995). Immediately after “surface activation”, the wafers can be placed together to form strong bonds at room temperature.

One may contrast the two technologies, sintering of ceramic powders, and bonding of semiconductor wafers. Both require geometric and chemical changes, but to different degrees. In powder sintering, the change from a porous to a dense body can never be accommodated by elasticity, but requires mass diffusion at high temperatures. In wafer bonding, it is relatively easy to polish surfaces so flat that misfit can be accommodated by elasticity, so that only a moderate temperature is needed to activate the chemical changes involving the adsorbed molecules. Consequently, the heat treatment temperature is set by geometric change in powder sintering, but by chemical changes in wafer bonding if wafers are well polished. The criteria given in this paper dictates how well the wafers need be polished.

Our model assumes that, after bonding, the shear stresses on the interface vanish, and the misfit is accommodated by the elastic displacements normal to the interface. The assumption appears to be reasonable for identical materials. For bonding dissimilar crystals, the stress state at the interface depends on the atomic arrangement. As mentioned before, when InP and GaAs wafers are bonded, arrays of dislocations

lie on the interface to offset the difference in lattice constants. The shear stresses on the interface certainly do not vanish in this case. Our model should be extended to include this feature. In using our model in its present version, one may consider the case where the wavelength of nonflatness is much larger than the spacing of the misfit dislocations, and include the elastic energy induced by the misfit dislocation into the interfacial energy, γ_{12} . Liao (1997) described a model for stress field generated by misfit dislocations alone. It gives reasonable stress field at a distance comparable to the dislocation spacing, but is inapplicable near the dislocations. He did not consider the misfit due to nonflatness of the surfaces, or the critical condition for bonding.

Our model assumes that the misfit has only one wavelength. In practice, the misfit contains many wavelengths, each having its own amplitude. One can perform a Fourier transform to obtain the misfit magnitude as a function of wavelength. The stress field due to misfit of each individual wavelength can be obtained by the procedure used in this paper, and the total stress can be obtained by linear superposition. The strain energy in the wafer can also be computed. The bonding criterion so established will be more rigorous, but harder to grasp. Instead, one may treat the problem approximately as follows. Consider the limit where wavelength is much smaller than the thickness of either wafer, and the present model gives bonding criterion (27). Of all the misfit wavelengths, the one having the largest ratio H^2/L is most difficult to accommodate. Consequently, one may use this wavelength in using the present model.

CONCLUDING REMARKS

Two wafers can adhere spontaneously if (a) the Dupré work of adhesion is positive, and (b) the shapes of the two surfaces sufficiently match. The work of adhesion can be modified by chemical reactions at the interface. When one has to bond wafers without the aid of mass transport or plastic flow, elastic distortion may accommodate a small amount roughness. For a given misfit wavelength, eqn (24) gives the maximum misfit height that can be accommodated elastically. The stress field in the bonded wafers due to misfit is localized near the interface, in a region of a thickness scaled with the misfit wavelength. The model does not specify the bonding type. Consequently, it applies to all the variations of the wafer bonding technique, including optical contact formed at room temperature due to van der Waals or other weak bonds, strong bonds formed at the room temperature after "surface activation" prior to bonding, and strong bonds obtained by changing weak bonds at a moderate temperature where mass transport is negligible. We obtained analytical expression for two layers of arbitrary thickness and elastic constants, so that thin film lift-off technique can be considered as a special case. We have only considered mechanical property of the bonded wafers in this paper. Depending on applications, one expects that chemical, optical, electrical, and optoelectronic properties can also be important. It would be interesting to study the effect of misfit on these properties. Furthermore, intentionally patterned misfit may lead to novel devices, where the interplay of adhesion and elasticity should play an equally important role. In this connection, it would be useful to analyze the extent of bonding when the surfaces do not close completely.

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