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DIE BOND MATERIALS AND BONDING MECHANISMS IN MICROELECTRONIC PACKAGING*

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The bonding mechanism for a silver–lead borate glass adhesive, used as a die bonding material in microelectronics packaging, was investigated. Silicon dies were bonded to alumina substrates with the glass adhesive, thermally cured and then sectioned, polished and analyzed. The diffusion of silicon from the die was found to be important in the development of the bond. Adhesion between the silver glass and the silicon die was found to be achieved via a glass network structure that starts at the silicon dioxide film on the die back side. Bonding between silver glass and the ceramic substrate was found to be mechanical in nature.

1. INTRODUCTION

One important aspect of reliability issues in microchip packaging is the extent to which the chip is securely fastened to the package, thus enabling the two to perform as one cohesive unit. The die bonding process, including the die bond materials used, controls this cohesiveness. Ideally, die bonds should be capable of holding the microchip onto the package reliably over the lifetime of the device. There are several factors that affect the adhesive's ability to fulfill this requirement. The die bond materials used, the corresponding bonding mechanisms that provide the adhesion and the variety of factors that can lead to bond failure are reviewed in this paper. The experimental investigation performed to determine the bonding mechanism for a silver-loaded lead borate glass adhesive and the role played by silicon diffusion in the bonding are also described.

All bonded devices constitute two adherands with an adhesive in between. This therefore contains two boundary layers or interfaces, as shown in Fig. 1. Failure can occur at one of three areas, namely the two boundary layers or the adhesive layer. Failure of the boundary layer is adhesive failure and failure of the adhesive itself is cohesive failure. As the adhesive layer gets thinner, the probability of its failure decreases, with a resultant increase in the importance of the boundary layers.

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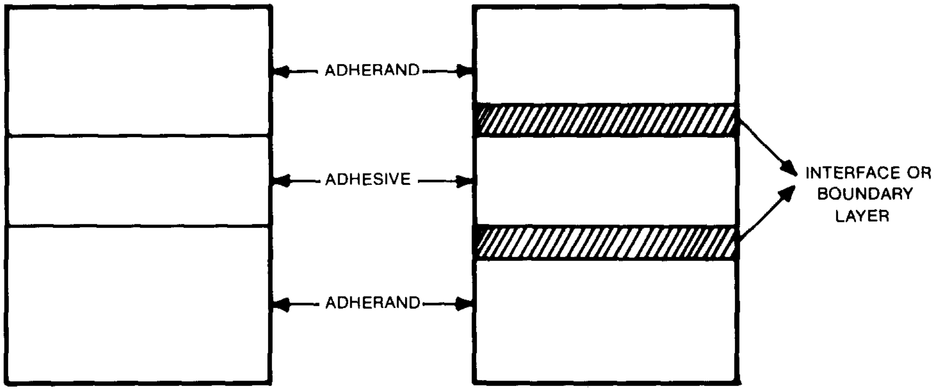


Fig. 1. Schematic diagram showing adherands and adhesives with interface between them.

Further, since the boundary layers constitute an interface, it is this area that generally contains extraneous factors that can affect long-term reliability.

In this paper, therefore, we concentrate on the interfaces, and address issues pertaining to adhesion rather than cohesion. The types of interfaces for a silicon die on a ceramic substrate with gold metallization are shown in Table I.

TABLE I
INTERFACE TYPE AS A FUNCTION OF DIE BONDING MATERIALS

Adhesive type	*Die side*	*Package side*
Solders	Metal–metal Metal–oxide	Metal–metal
Organic	Organic–metal Organic–oxide	Organic–metal
Glass	Oxide–metal Oxide–oxide	Oxide–metal

2. DIE BOND MATERIALS

Die bonding materials can be classified into three major categories: (a) eutectic die bonds, (b) organic adhesives and (c) glass adhesives.

2.1. *Eutectic die bonds*

Also known as solders, eutectic die bonds are generally binary or ternary metallic compositions which exhibit positive deviation from ideality. Solders are divided into hard solders and soft solders. The higher melting point solders, or hard solders, have higher yield stresses and are used where service temperatures are higher. Non-lead-based hard solders include Au–Si, Au–Sn and Au–Ge. Soft solders, in contrast, have low melting temperatures and lower yield stresses. The solidus and liquidus temperatures of a number of solder compositions are summarized in Table II[1]. Eutectic solder alloys are typically supplied as a preform or in ribbon form, and are generally recognized as the most reliable bonding–sealing material, even though they are the most expensive. The systems most commonly used in die attach applications are Au–Si, Au–Ge, Au–Sn, Pb–Sn and Pb–In–Ag [2].

TABLE II

COMPOSITIONS AND MELTING POINTS FOR DIE BOND PREFORMS[1]

Composition (wt.%)	*Temperature* (°C)	
	Liquidus	*Solidus*
80Au–20Sn	280	280
92.5Pb–2.5Ag–5In	300	
97.5Pb–1.5Ag–1Sn	309	309
95Pb–5Sn	314	310
88Au–12Ge	356	356
98Au–2Si	800	370
100Au	1063	

2.2. *Organic adhesives*

Silver- and gold-filled epoxies and polyimides are used widely as die bond materials in low cost plastic packages[2]. The epoxy adhesives which contain approximately 70% metallic fillers to provide the required electrical and thermal conduction are generally a low viscosity thixotropic paste in a heat-curing binder. They are most commonly the condensation products of epichlorohydrin and bisphenol A (4,4′-isopropylidene diphenol)[3], although several other proprietary formulations exist. Most varieties contain a solvent. There are a number of varieties that are one-part and/or solvent free[4].

Polymers incorporating the imide group in the polymer main chain and derived from aromatic acids have aroused particular interest in recent years because of their outstanding thermal stability. These polymers, called polyimides, are a newer class of organic adhesives that are used for chip bonding. Like the epoxy adhesives, polyimide adhesives also contain approximately 70% silver powder as a filler.

2.3. *Glass adhesives*

Low melting lead borate and lead borosilicate glasses have been used as a glass–metal adhesive for a considerably long time[5]. These have relatively low glass transition and working temperatures. In microchip packaging, however, silver-filled lead borate glass is a new adhesive and is gaining in popularity. Silver is added to improve thermal and electrical conductivity.

3. EFFECT OF DIE BOND ON MICROCHIP RELIABILITY

The two main concerns are chip disbonding and chip cracking. Both of these issues are affected by the characteristics of the adhesive used. Although there are a large variety of factors that affect the role die bond materials play in reliability issues, not only are these too numerous but also several of these factors are unique to specific die bond–die combinations. As such, only the major issues having general relevance are discussed here.

Thermal stability of the die bond material is of paramount importance because of the requirement to withstand subsequent high temperature processes such as wire bonding and/or sealing. Cerdip packages, for example, are sealed in air at 420–450 °C. Most of the epoxy adhesives are at a major disadvantage here since they cannot withstand temperatures much higher than 300–400 °C without degradation. Polyimides have far better high temperature stability, compared with epoxies. Thermogravimetric analyses of polypyromellitimides indicate that they remain stable to over 500 °C in vacuum or inert atmosphere[6]. The Au–Si bonds which are made at 430 °C have a distinct advantage here. However, some of the other lower melting solders do not necessarily have any advantage over the organic adhesives. The silver glass adhesive is quite stable in air to relatively high temperatures because its components are oxides.

In addition to containing the microchip and facilitating handling, the package is also designed to serve as a heat sink, and the adhesive must therefore be conductive. Of the three classes of adhesives, only solders are naturally conductive (thermally and electrically). Organic and glass adhesives need a metallic filler to impart the required conductivity characteristics to them. Although in theory any metallic powder could serve this purpose, in practice the powders should not be oxidized by the adhesive; hence noble metal powders such as gold, silver or platinum are desirable. Silver is the cheapest. In order to provide a conductive path the powders should be connected, which requires them to be not only finely divided but also contained in sufficient quantities. On the basis of this requirement we find that the silver content in the organic and glass adhesives is approximately 70 wt.%.

The service temperature requirements are usually from −40 to +140 °C. Mismatches in thermal expansion cause thermal stresses to be set up. The extent to which such stresses are induced in the die is a function of the mismatch in thermal expansion between the die and the adhesive. Induction of stresses in the die due to mismatch between the die and the package is a function of the shear strength of the adhesive. Those adhesives with lower shear strengths will be less prone to causing stresses in the die.

The fatigue lives of adhesives are also dependent on their shear strength, in addition to ductility. In evaluating resistance to fatigue, it is important to distinguish between mechanically induced stresses and stresses arising from thermal cycling. The stresses caused by an increase in temperature are frequently less important because of (1) the accompanying drop in elastic modulus and (2) the tendency of most solders to recrystallize, provided that sufficient time is available. Under thermal cycling conditions, fatigue endurance is strongly dependent on both the range of temperatures between which the device is cycled and the actual temperature level and specific time–temperature cycle. The temperature of recrystallization is approximately one-half the liquidus temperature. Higher melting point solders would therefore be less capable of recrystallizing and would therefore be more prone to fatigue failure. Creep failure, however, would increase with lower liquidus temperatures.

The presence of solvents in the adhesives usually poses the problem of residual porosity after curing. Solvents are employed with both organic as well as glass adhesives, and they provide the fluidity necessary for dispensing. Residual porosity has been found to result in a bond with inferior mechanical, electrical and thermal performance[7].

The presence of ionic impurities, particularly chlorides, and moisture also has a detrimental effect on long-term integrity. The presence of moisture has been known to affect the long-term stability of adhesives[8]. One of the main ions of concern is Cl^- which in combination with the moisture present forms HCl, thus leading to corrosion problems and failure.

4. BONDING MECHANISMS

4.1. *Thermodynamics of adhesion*

The work W_{AB} of adhesion can be expressed as

$$W_{AB} = \gamma_A + \gamma_B - \gamma_{AB} \tag{1}$$

where γ_A is the surface tension of body A, γ_B is the surface tension of body B and γ_{AB} is the interfacial tension between the two bodies. The driving force for adhesion is thermodynamic in nature, and if two bodies can lower their total free energy by "uniting" then they can be considered to have adhered.

In order for a liquid to adhere to a solid surface, and thereby to lower the overall free energy of the system, "wetting" is essential. Basic to the concept of wettability is Young's concept of the contact angle θ between a drop of liquid and a plane solid surface. This is illustrated in Fig. 2 where θ is the wetting angle, γ_L is the surface tension of the liquid, γ_S is the surface tension of the solid, and γ_{LS} is the interfacial surface tension.

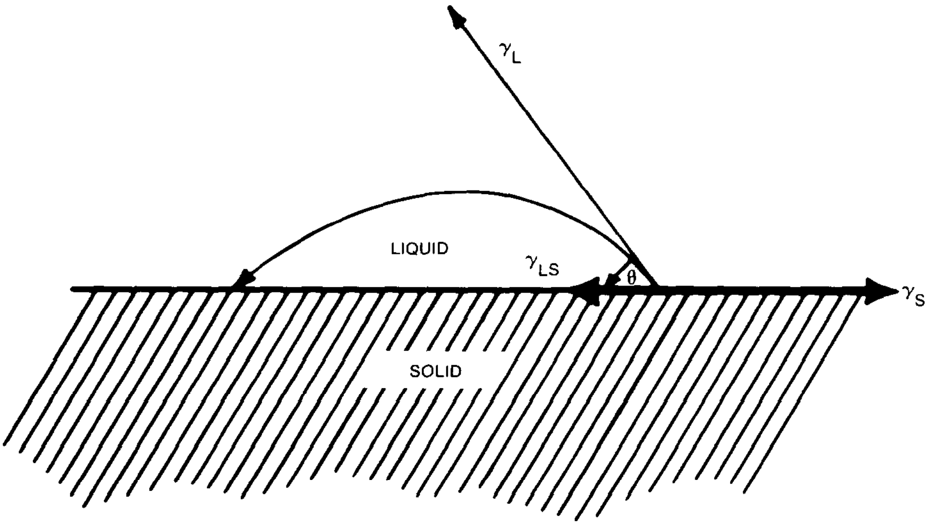


Fig. 2. Surface tension forces involved in wetting of a substrate by a liquid.

When the wetting angle θ is less than 90° the liquid wets the solid surface. In order for equilibrium to exist, the following condition must be satisfied:

$$\gamma_{LS}+\gamma_L \cos\theta = \gamma_S \tag{2}$$

where θ varies from 0° to 180°. From this formulation it can be shown that (1) the surface tension of the solid must be greater than the surface tension of the interface and (2) the surface tension of the liquid–solid interface must be greater than the difference between the surface tensions of the solid and the liquid.

When the contact angle θ approaches zero, then $\gamma_S = \gamma_L$ and the interfacial tension becomes zero.

4.2. *Eutectic die bonding mechanisms*

Solders act by the following sequential steps: (1) wetting the substrate surfaces, thus forming the joint; (2) flowing between these surfaces so as to fill completely the space between them; (3) metallurgically bonding to the surfaces when solidified[9].

When silicon chips are attached to ceramic packages with gold-plated chip pads, the eutectic die bonding material is Au–Si. The phase diagram for this system is shown in Fig. 3[10]. Typically, the package is heated to above the eutectic temperature (363 °C) and then the chip is scrubbed onto the gold until an alloy is formed. The use of Au–Si eutectic preforms or pure gold preforms to initiate the reaction and to improve the bonding is also not uncommon[11].

Gold and silicon when alloyed exhibit positive deviation from ideality. Although the individual elements melt at 1063 °C and 1412 °C respectively, their

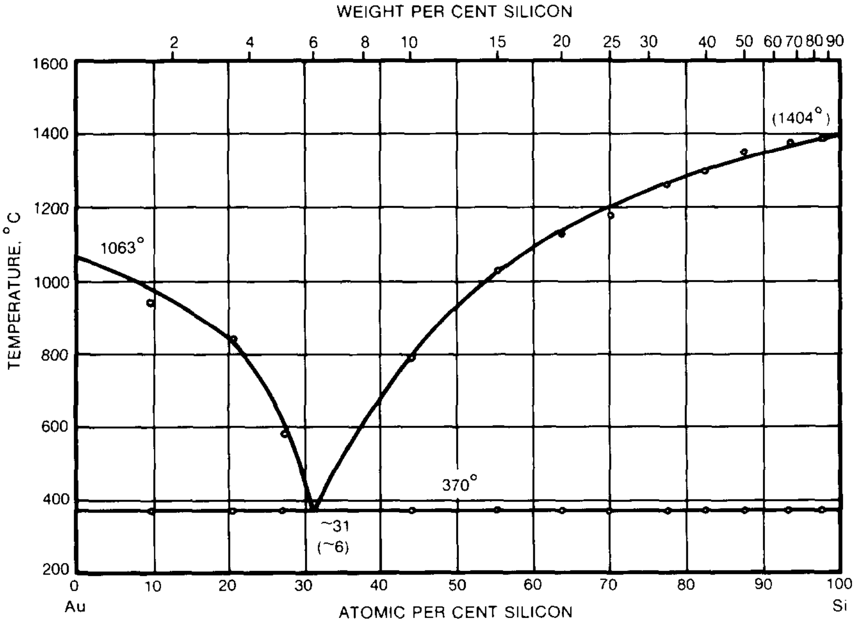


Fig. 3. The Au–Si phase diagram[10].

eutectic temperature of 363 °C represents one of the most dramatic reductions in the melting point of any combination of the common elements.

At typical bonding temperatures of greater than 400 °C a liquid phase exists, with the equilibrium composition varying between 18% and 25%. If a preform is used, silicon from the die back side and gold from the substrate are consumed in order to achieve equilibrium.

On cooling the bonding is provided specifically by the eutectic reaction:

$$L = Au(s) + Si(s) \tag{3}$$

which leads to the formation of two solid phases, interlocking and providing the required continuity into the silicon die and the gold-plated chip pad.

Because of the extreme thermodynamic stability of SiO_2, the silicon die can logically be expected to have an SiO_2 layer on the back side. Scrubbing of the chip during the die bonding process helps to break away these oxide layers as well as to remove other contaminants so that a clean silicon surface can be exposed for bonding[12]. Scrubbing also helps to homogenize the liquefied interface, minimizing segregation.

Prolonged use at high temperatures can be expected to weaken the bond formed via solid state diffusion of gold to gold and silicon to silicon. This results in segregation of the two elements, thus breaking down the interlocking phases that had been formed. The silicon contained in the Au–Si eutectic die bond runs the risk of being oxidized, thus degrading the integrity of the bond.

The oxidizing mechanism of Au–Si alloys was studied in depth, with Rutherford backscattering, by Mayer[13]. His model is shown in Fig. 4. This study

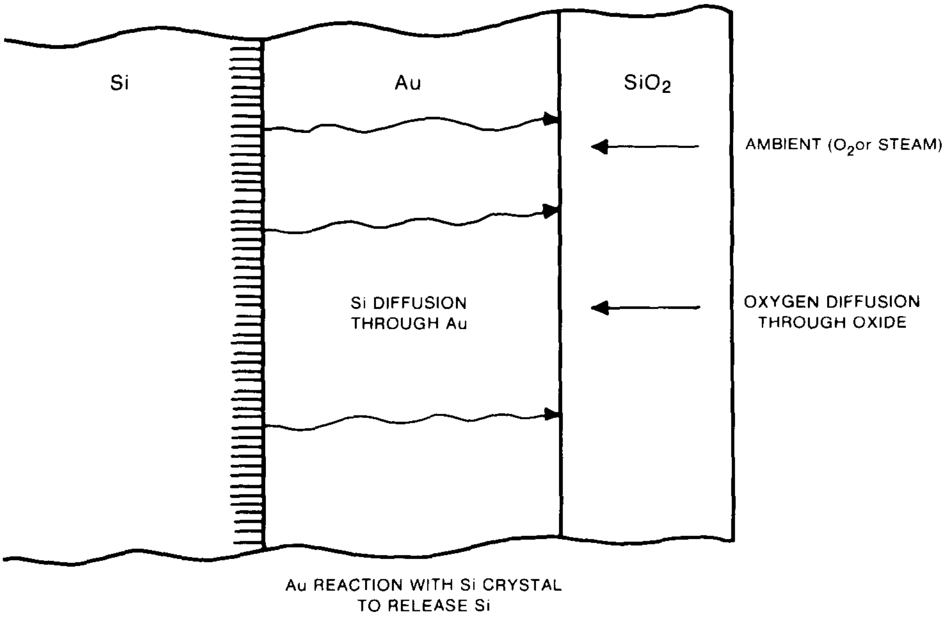
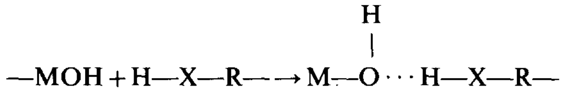


Fig. 4. Oxidation mechanism of the Au–Si interface[13].

indicates that silicon diffuses through the gold layer to react with ambient oxygen, thus forming the oxide at the Au–SiO_2 interface. Because of the high diffusivity of silicon in gold, and of oxygen through the porous SiO_2 layer, the reaction occurs at this interface. Although the gold reacts with the silicon here, to release the silicon atoms for migration, the interface itself is not affected by the oxygen. This can be ascribed to the extremely low solubility of gaseous oxygen in gold.

4.3. Organic adhesive bonding mechanisms

The bonding mechanism between high energy solid surfaces such as those formed by metals, metal oxides and silicates and polymeric adhesives has been described in detail by Kaelble[14] and is summarized here. Most metal surfaces have oxide layers of 40–80 Å thickness, which at ambient conditions is hydrated to present a high density of hydroxyl groups. This hydroxylated oxide layer readily adsorbs and strongly retains a multimolecular layer of physically adsorbed water. Bolger and Michaels[15] point out that different metals, oxides and silicates display differing types of interaction with organic adhesives, and they elucidate many of the distinguishing features of these specific interactions in terms of the ionic character of the hydroxylated substrate and the organic functional group provided by the adhesive. The four generalized types of acid–base reactions which involve the hydrated oxide surface and organic acids or bases are as follows:



$$\text{—MOH} + \text{H—X—R} \longrightarrow \text{M—}\overset{\overset{\text{H}}{|}}{\text{O}}\cdots\text{H—X—R—} \qquad (4)$$

$$\text{—MOH} + \text{H—X—R} \longrightarrow \text{—MOH}_2{}^{+}\text{X}^{-}\text{—R—} \qquad (5)$$

$$\text{—MOH} + \text{X—R} \longrightarrow \text{—MOH}\cdots\text{X—R—} \qquad (6)$$

$$\text{—MOH} + \text{X—R} \longrightarrow \text{—M—O}^{-}\text{H}^{+}\text{—X—R—} \qquad (7)$$

Reactions (4) and (6) describe hydrogen bond formation whereas reactions (5) and (7) describe ionic interactions.

4.4. Silver glass bonding mechanism

The bonding between the glass die attach and metallic die falls within the category of glass–metal bonds. In order for bonding to occur, the glass should spread on the metal and wet it. Even at higher temperatures, dispersion forces are insufficient to make glass spread unless an oxide is first formed on the metal[16]. Pask[17] reviewed the evidence on the interaction between glass and gold, platinum and iron and found the formation of a metal oxide essential. Wetting equilibrium is dependent on (i) the solubility of oxygen in the metal, (ii) the solubility of the metal oxide layer in the glass and (iii) the rate of oxygen diffusion to the interface.

The characteristics of the bond formed by a commercial silver glass adhesive with a silicon die on one side, and a gold-plated substrate on the other side, were studied experimentally. As can be seen from the PbO–B_2O_3 phase diagram shown in Fig. 5 (ref. 18, p. 115), the lowest melting eutectic in this system has the composition 88 wt.% PbO and 12 wt.% B_2O_3 and melts at 493 °C. The lead-rich side of the PbO–B_2O_3–SiO_2 ternary phase diagram is shown in Fig. 6 (ref. 18, p. 254).

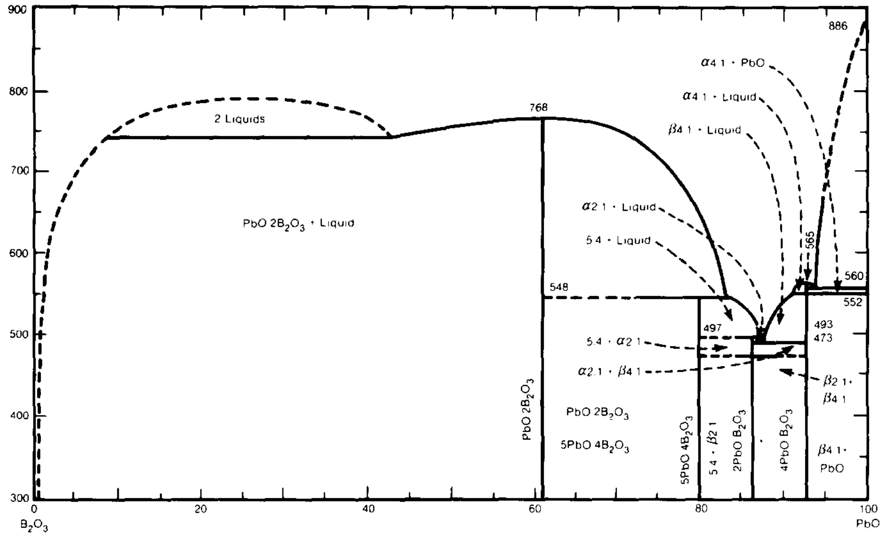


Fig. 5. The $PbO-B_2O_3$ phase diagram (ref. 18, p. 115).

The incorporation of SiO_2 into the $PbO-B_2O_3$ system lowers the eutectic temperature slightly to 484 °C. However, what is more interesting is the formation of a solid solution at SiO_2 concentrations of around 8 wt.%.

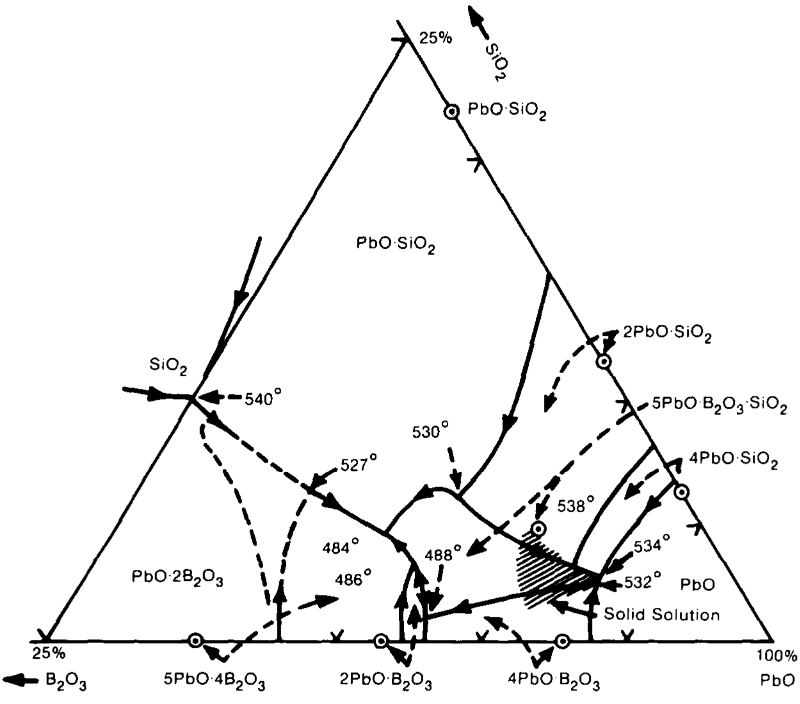


Fig. 6. Lead-rich side of the $PbO-B_2O_3-SiO_2$ ternary phase diagram (ref. 18, p. 254).

Unlike metallic alloys, which exhibit liquefaction at fixed temperatures and have physical properties that vary discontinuously at these temperatures, glasses transform from the solid to the liquid phase gradually. The variation in physical properties is accordingly gradual, as is shown in Fig. 7. Lead borate systems having a PbO composition of 90 wt.% begin to soften at 286 °C (ref. 19). The significance of the onset of softening is that the viscosity begins to decrease, thereby permitting increased atomic mobility for adhesion.

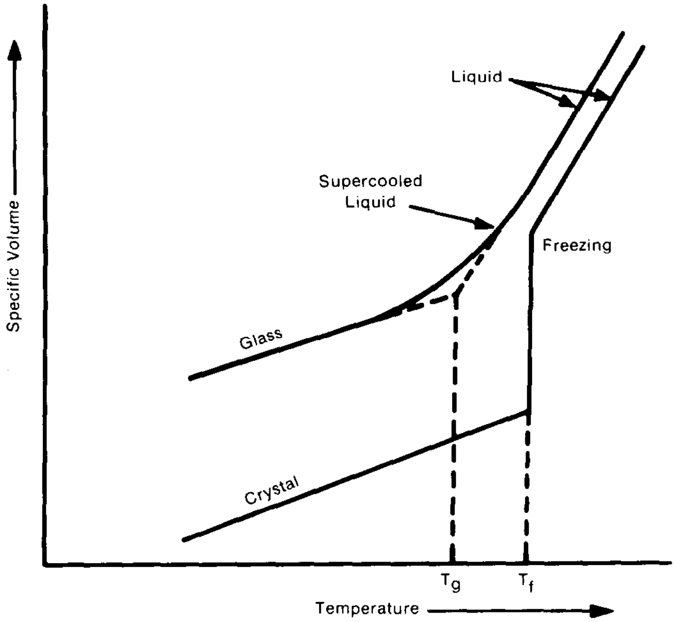


Fig. 7. Liquid–solid transition, as illustrated by the specific volume, for an amorphous glass and for a crystalline solid.

Silicon dies were bonded to alumina substrates with gold metallization and processed according to the schedule shown in Fig. 8. The samples were sectioned, mounted in Araldite and polished before microanalysis by energy-dispersive spectroscopy. These analyses were carried out across the silicon–silver glass interface and the silver glass–gold interface and also from the silicon die across the silver glass die bond and into the substrate to detect the presence and relative amounts of each element at various depths. In each of these cases the sample was scanned for the intensity of characteristic X-rays. The results are shown in Figs. 9–11. It is evident from Fig. 9 that silicon diffuses into the silver glass die bond layer and penetrates it to about one-half of its thickness.

An important point in the discussion of the bonding mechanism between silver glass and the die is the presence of a layer of silicon dioxide on the die back side (unmetallized die). This oxide layer plays an important role in the bonding mechanism.

On curing the packaged die at approximately 430 °C, the lead borate glass

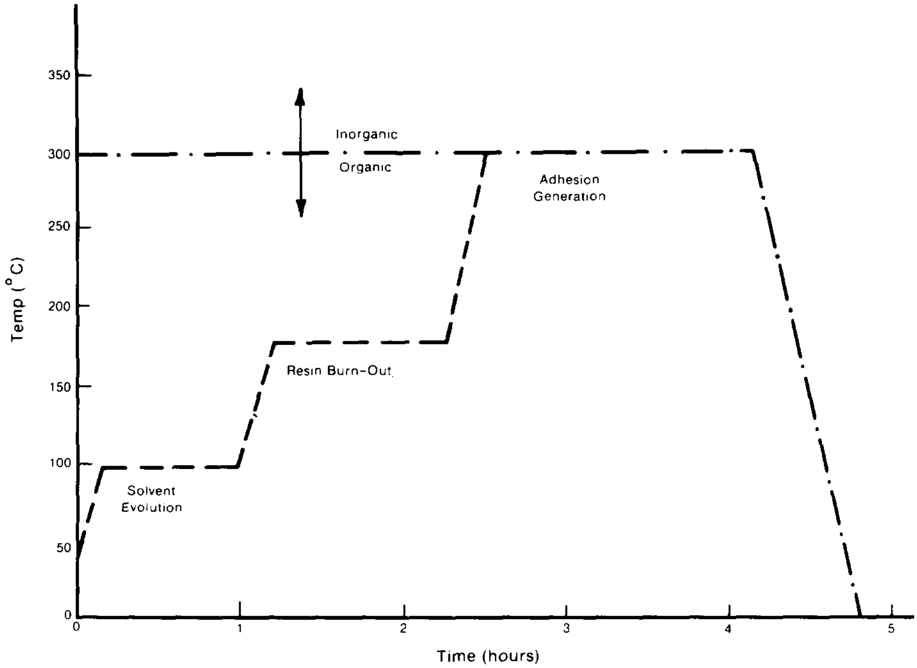
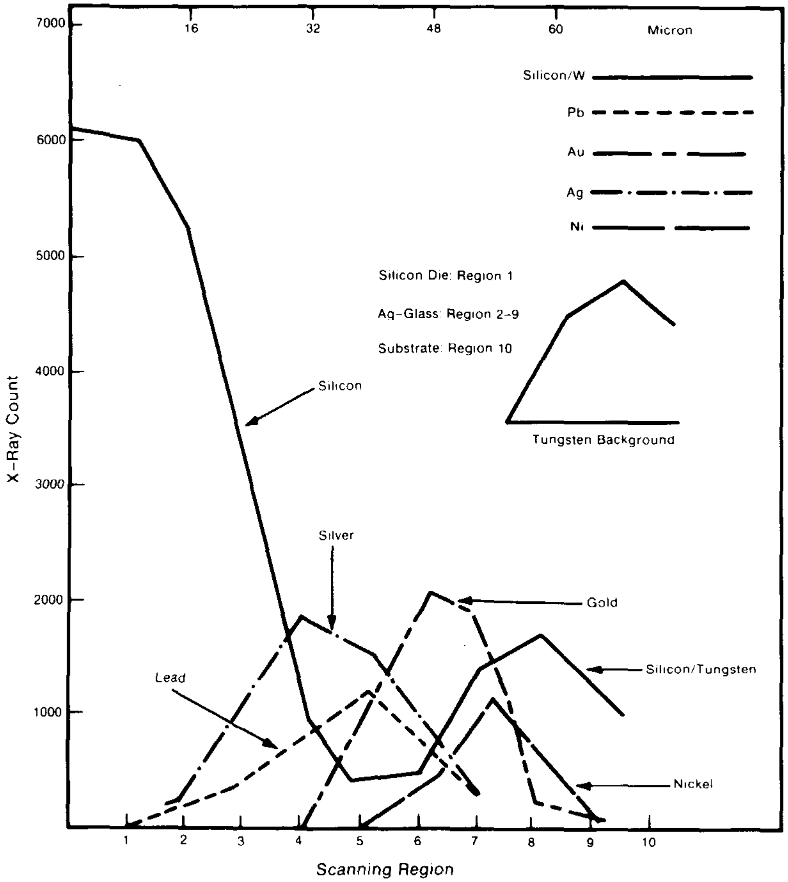


Fig. 8. Processing cycle of silicon die bonded to gold-metallized alumina substrates using a silver glass die bond.

comes in contact with silicon dioxide. B_2O_3, which is a glass former in its own right, acts as a fluxing agent for SiO_2 in this case, thereby reducing its melting temperature[20]. Figure 12 shows the phase diagram for the system B_2O_3–SiO_2 (ref. 21). A multicomponent glass is therefore formed at the silicon die–silver glass interface. The system PbO–B_2O_3–SiO_2 (Fig. 6) shows two eutectics with compositions close to what is expected to be present at the silicon–silver glass interface. These are 84 wt.% PbO, 11 wt.% B_2O_3 and 5 wt.% SiO_2, with a eutectic temperature of 484 °C, and 93 wt.% PbO, 5 wt.% B_2O_3 and 2 wt.% SiO_2 at 532 °C.

During bonding of the die back side and silver glass, the SiO_2 layer on the die back side softens at processing temperatures because of its contact with the lead borate glass. The silica crystalline structure close to the interface is interrupted and some Si—O bonds that join the SiO_4 tetrahedra together are broken. Some of the silicon from the die back side enters the lead borate network by sharing oxygen atoms with boron and lead. Compositions near the ternary eutectic are reached and bonding takes place via a eutectic reaction. The system will have a complex network structure with silicon, boron and lead as network formers and some of the lead cations will fill the holes in the network. The unreacted glass forms an interlaced network with silver. The presence of SiO_2 on the die back side is essential for adhesion.

The other end of the bonding process is the adhesion between the die bonding material and the gold-covered substrate. The presence of gold inside the die bond layer has been documented in Figs. 9 and 11. The analysis of the interface shows that



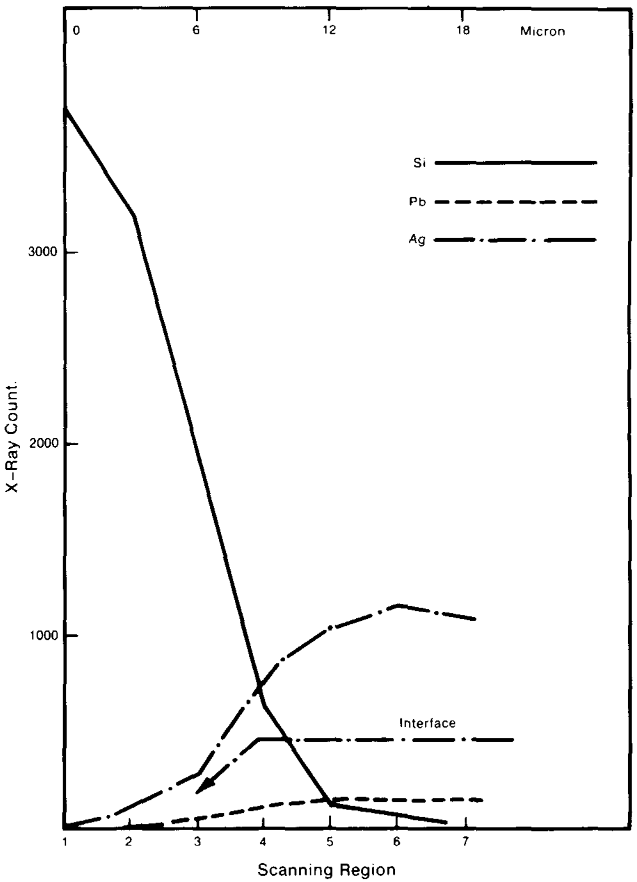


Fig. 9. Variation in X-ray intensity of constituent elements from the silicon die (region 1) to the substrate (region 10).

Fig. 10. Variation in X-ray intensity of constituent elements across the Si–Ag glass interface.

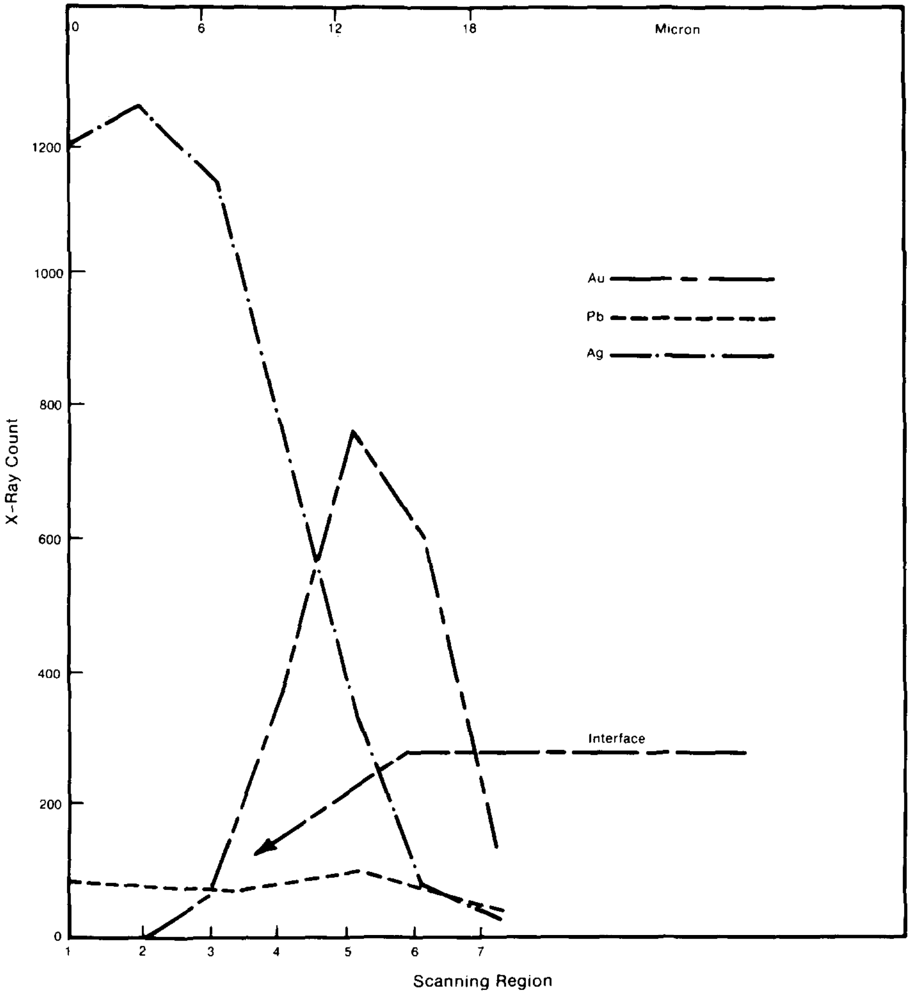


Fig. 11. Variation in X-ray intensity of constituent elements across the Ag glass–Au interface.

both gold and silver glass interdiffuse to make the bond that adheres the two together. The nature of this bond, however, is completely different from that previously discussed between the die and the die bond. Gold diffuses through the network structure during the process cycle and silver glass paste seeps through the surface imperfections in the gold film to the pores in the ceramic substrate, resulting in a mechanical bond between the gold and the glass.

5. CONCLUSION

A large number of factors come into play in deciding the long-term reliability of die bonds. These are invariably dependent on the specific type of die in question, the particular package being used and the adhesive utilized. An understanding of the

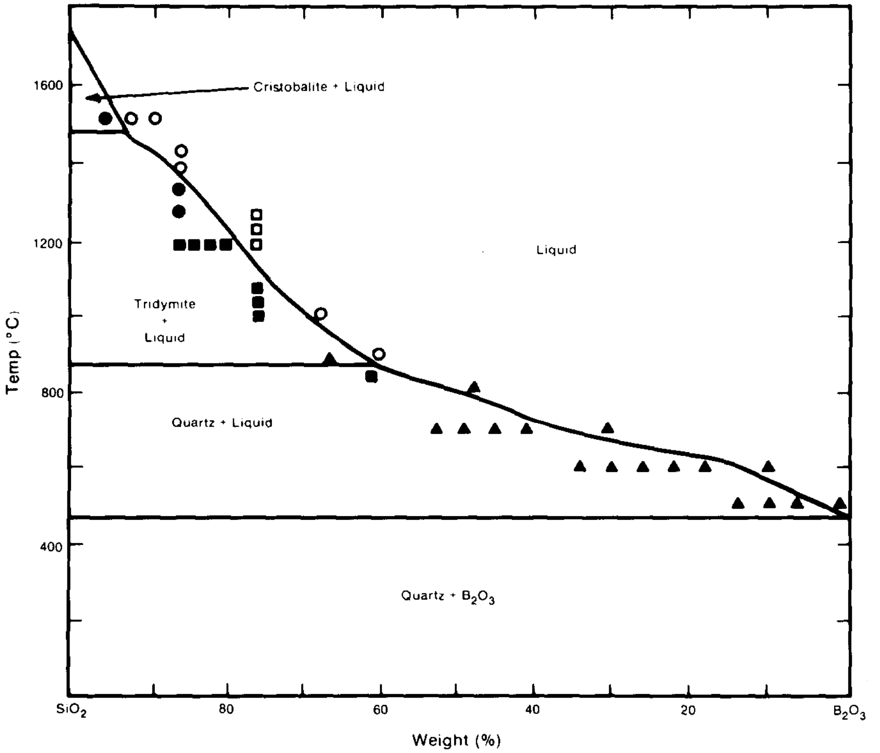


Fig. 12. The B_2O_3–SiO_2 phase diagram[21].

mechanism(s) via which various adhesives provide the required adhesion will help in the selection of appropriate die attach materials for particular chip–package combinations. The formation of an SiO_2 layer on the back side of an unmetallized die, for example, has been found to be essential for bonding with silver glass adhesives.

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