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Scripta Materialia 66 (2012) 694–697
Scripta MATERIALIA
www.elsevier.com/locate/scriptamat

Thermomigration of Ti in flip-chip solder joints

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Received 9 November 2011; revised 13 January 2012; accepted 16 January 2012
Available online 21 January 2012

Titanium has a very large heat of transport value of −768 kJ mol^{-1}. However, thermomigration of Ti in solder joints has not been examined. In this study, void formation was observed in non-current-stressed Al traces during electromigration and thermomigration tests of SnAg solder joints. Voids formed inside the traces located above the solder bumps with no current flow. We found that Ti thermomigration occurred in the joint, resulting in the reaction of Al and Cu, leaving voids behind in the Al trace.
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Keywords: Diffusion; Intermetallic compounds; Soldering; Titanium

Owing to the continuous trend of down-scaling and the increasing demand for high-performance electronics devices, the current density in devices and interconnects continues to increase. Electromigration has also become a critical reliability issue [1–5]. During high-current-density stressing, non-uniform heating takes place in solder joints, resulting in thermomigration damage [5–10]. In recent years, thermomigration in flip-chip solder joints has attracted much attention. Since Al traces serve as the major heat source during accelerated electromigration tests, a non-uniform temperature distribution is generated, resulting in a large thermal gradient across flip-chip solder joints [11]. This thermal gradient has been demonstrated to induce thermomigration during accelerated electromigration tests [6,8,9]. Many studies have been conducted in order to better understand this reliability issue in solder materials [6–14]. Pb atoms tend to migrate to the cold end along the thermal gradient, while Sn atoms tend to migrate to the hot end. It has also been reported that thermomigration can occur in the Cu layer of an under-bump-metallization (UBM) structure [13], where Cu moves to the cold end under a thermal gradient. Among the materials used for UBM structure, Ti has been widely adopted as the diffusion barrier between the Al trace and the Cu UBM. It is reported that Ti has a very large heat of transport value of −768 kJ mol^{-1} [15,16] and is liable to migrate under a thermal gradient. However, no study has been performed to examine the thermomigration of Ti in solder joints.

In this study, thermomigration tests were performed in flip-chip solder joints with Cu/Ti UBMs where Ti acts as a diffusion barrier. Extensive voids were formed in the Al trace with no current stressing. It is found that thermomigration of Ti atoms causes damage in the diffusion barrier layer, and Al subsequently migrates into the Cu UBM. Simulation results reveal a large thermal gradient across the Ti layer, which induces thermomigration of Ti atoms from the hot end toward the cold end. Theoretical calculations were also conducted to confirm the observed phenomena.

Cross-sectional studies of solder bumps were employed to facilitate the observation of both electromigration and thermomigration damages. The test layout is shown in Figure 1a. Figure 1b shows the dimensions and microstructures of the SnAg3.5 flip-chip joints used in this study. The width and height of the bumps are 130 μm and 75–80 μm, respectively. On the chip side, a 0.12 μm thick Ti layer was sputtered as an adhesion/diffusion-barrier layer between the Cu UBM and the Al trace. The solder joints comprised eutectic SnAg solder bumps and 5 μm electroplated Cu UBMs, as shown in Figure 1b. The electromigration test layout consisted of four bumps and an Al trace connecting them. This test layout provided Kelvin bump probes that can facilitate highly precise measurement of bump resistance [17]. An electric current of 0.55 A was applied through nodes

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doi:10.1016/j.scriptamat.2012.01.020

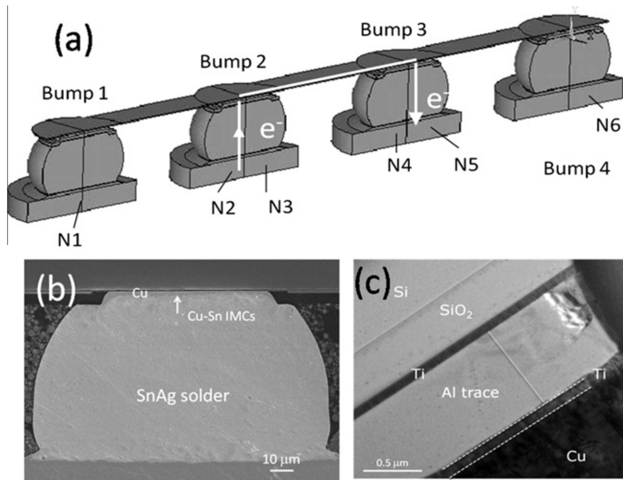

Figure 1. (a) Cross-sectional schematic of the test layout. An Al trace connected all the four solder bumps together. Cross-sectional SEM image showing the microstructure of the solder bump used in this study with (b) a 5 μm Cu UBM and (c) cross-sectional TEM image showing Al trace, Ti layer and Cu UBM structure before current stressing.

N3 and N4, producing a nominal current density of 9.7×10^3 A cm^{-2} in Bump 2 and Bump 3 and 7.3×10^5 A cm^{-2} in the Al trace. However, the four bumps experienced similar amounts of Joule heating because they are connected together by the Al line on the Si die; both materials are known to be excellent heat conductors. Figure 1c shows a cross-sectional transmission electron microscopy (TEM) image of the interface of the Al trace and the Cu UBM in the as-fabricated sample. A Ti diffusion barrier of 0.12 μm thick exists between the Al trace and the Cu layer and is shown by the dotted line in the figure. This layer adhered quite well to the Al and Cu films before thermomigration tests. The corresponding diffraction patterns for the Ti and the Al layers are shown in the Supplementary Material. No voids could be observed in the structure. There was another Ti layer between the SiO_2 and the Al trace layer. However, this Ti layer was not damaged during thermomigration tests. This Ti layer was denoted as the first Ti layer while the other was denoted as the second Ti layer. The Al trace on the chip side was 100 μm wide and 1.0 μm thick. After current stressing, the surface morphology of the joint was observed by scanning electron microscopy (SEM) and the compositions of the solder joints and the intermetallics (IMCs) were analyzed quantitatively by energy dispersive spectroscopy (EDX). To observe the microstructure on the Al/Ti/Cu interface, a focused ion beam (FIB) was adopted to etch a second cross-section around the interface between the Si die and the solder to analyze the damage after thermomigration tests. Furthermore, TEM specimens were prepared by FIB. Three-dimensional (3-D) finite-element modeling was performed to analyze the temperature distribution across the interface because no experimental methods could be utilized to measure the actual temperature distribution in 1.0 μm thick Al traces.

Surprisingly, while there is no current flowing through Bump 1 and Bump 4, void formation occurred in the Al trace above these two bumps. Figure 2a shows the SEM image of the interface between Si and the solder in Bump 4. A current of 0.55 A was applied through Bump 2 and Bump 3 at 150 °C for 82 h. Bump 1 and Bump 4 experienced similar Joule heating effects as Bump 2 and Bump 3. Although there was no current flow in these two bumps, a thermal gradient exceeding 1000 °C cm^{-1} might build up in the solder and thermomigration could take place in Bumps 1 and 4 [13]. Some voids were observed in the Al trace and in the Cu–Sn interfacial IMCs after the thermomigration test for 82 h, as shown in Figure 2a. Furthermore, the Ti layer between the Al trace and the UBM disappeared after the test. Figure 2b presents the FIB ion image of the interface with the Cu–Sn IMCs more clearly illustrated. The first Ti layer stayed intact but the second Ti layer became discontinuous. As mentioned above, Cu is liable to migrate to the cold end, resulting in void formation at the original site of the Cu UBM [13]. However, serious void formation not caused by thermomigration of Cu was also observed in the Al trace, and hence there must be another mechanism responsible for the void formation. During thermomigration tests, the Si chip side served as the hot end and the substrate side acted as the cold end. Thus, the temperature in the Si chip was higher than that in the solder. It has been reported that Ti and Al have negative heat of transport values and they tend to move to the cold end under a thermal gradient [15,16,18]. Thus, thermomigration of Ti or Al may be responsible for void formation in the Al trace.

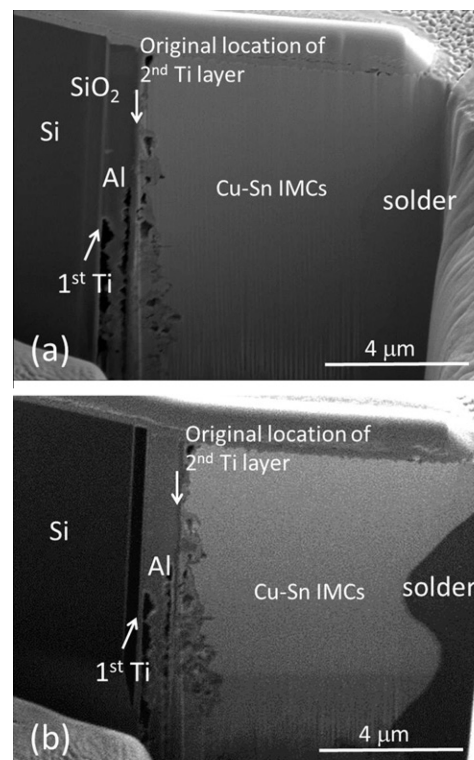

Figure 2. (a) Cross-sectional SEM image for Bump 4, showing microstructures at the interface of the chip and the solder after current stressing of 0.55 A through Bumps 2 and 3 at 150 °C for 82 h, and (b) FIB image for Bump 4 on the same area of (a).

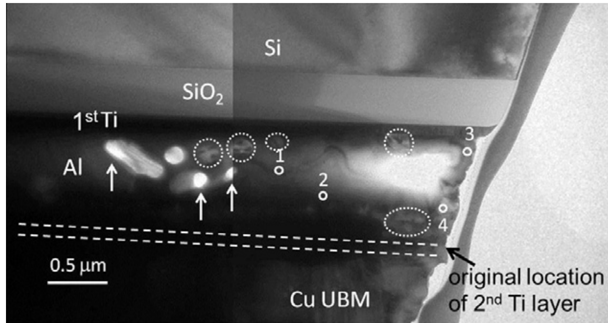

Figure 3. Cross-sectional TEM image of Al/Cu interface for Bump 4 after current stressing of 0.55 A through Bumps 2 and 3 at 150 °C for 82 h.

The results from TEM analysis indicate that Cu–Al IMCs formed after thermomigration tests. Figure 3 shows the cross-sectional TEM image of the damaged Al trace. Some voids formed in the Al trace, as indicated by the arrows in the figure. In addition, the second Ti layer between the Al and Cu layers disappeared. However, the first layer Ti layer remained continuous. TEM-EDX was performed to analyze the composition of the alloys and the IMCs near the Ti/Cu interface. Table 1 lists the results for the four points labeled in Figure 3. Some IMCs of Cu_9Al_4 were detected near the interface, as marked by the white-dotted circles. The above results suggest that thermomigration of Ti and Al may be mainly responsible for void formation in the Al trace. As shown in Figure 2a, the Al trace had no voids at the location where the Ti layer stayed intact. Once the Ti layer was destroyed, Al might then diffuse into the Cu UBM to form Cu–Al IMCs [16,18,19]. Hentzell et al. reported that Cu–Al reaction may take place at 200 °C for 1 h [20]. Once Al diffuses into the Cu UBM to form Al–Cu IMCs, void formation occurs in the Al trace. Therefore, the second Ti layer plays a critical role in void formation in the Al trace.

The thermomigration forces of Ti, Al and Cu are estimated, and Ti is found to have the largest value among the three elements. The thermomigration force is described as [21]:

$$F = -\frac{Q^*}{T}\left(\frac{\partial T}{\partial x}\right), \quad (1)$$

where T is the temperature, x is the distance and Q^* is the heat of transport. It has been reported that all these three materials tend to migrate to the cold end. Finite-element simulation was carried out to simulate the thermal gradient in Al/Ti/Cu layers. Figure 4a shows a schematic drawing of the model we used in the simulation. When electrons flow through Bump 2 and Bump 3, Joule heating occurs in the circuit and also heats up Bump 4. Therefore, a large thermal gradient is established in Bump 4. Figure 4b reveals the simulated temperature distribution along the solder bump defined by the dotted line shown in Figure 4a. The simulated points were started from the top of the Al trace and proceeded downward into the Cu UBM. The thermal gradient across the 1.0 μm thick Al trace is calculated to be 500 °C cm^{-1}. On the other hand, the thermal gradient across the second Ti layer is as high as 5800 °C cm^{-1}. This is reasonable because the Al trace serves as the main source of Joule heating and Ti has a low thermal conductivity of 46.1 W m^{-1} K^{-1}. Some of the heat dissipated downwards to the second Ti layer attached directly below the Al trace and into the solder bump. Thus, the second Ti layer may experience a larger thermal gradient than the Al trace and the Cu UBM. Ti possesses a very large heat of transport value of −768 kJ mol^{-1} toward the cold end [15,22] and is thus highly likely to migrate under a large thermal gradient. The thermomigration force is then calculated to be 1.75×10^{-17} N for Ti. The value of heat of transport for Al is taken to be −8.36 kJ mol^{-1} [15]. Thus, the thermomigration force is calculated to be 1.6×10^{-20} N for Al under the test condition in this study. On the other hand, the heat of transport value of Cu is −22.6 kJ mol^{-1} [15]. Therefore, the thermomigration force of Cu and Al have the same order of magnitude. The results indicate that Ti has the largest thermomigration force because it has the highest heat of transport value and the largest thermal gradient among the three elements. The force is approximately three orders of magnitude larger than that of Al and Cu.

Table 1. TEM-EDX compositional analysis for the four positions shown in Figure 3.

	Point 1	Point 2	Point 3	Point4
Al (at.%)	29.4	18.0	27.0	1.9
Cu (at.%)	70.6	56.7	73.0	18.7
Ti (at.%)	–	25.3	–	79.4

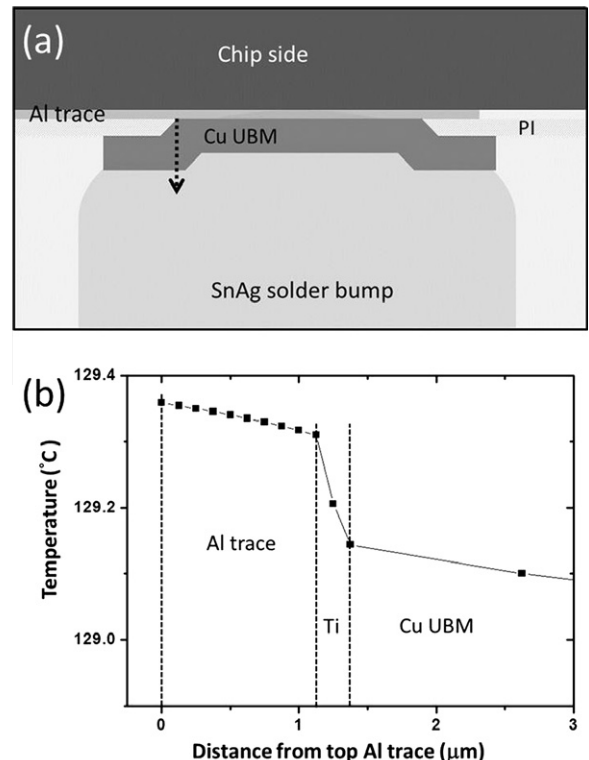

Figure 4. (a) Schematic structure of Bump 4 used for simulation. (b) Temperature distribution along the dotted line.

In this study, we propose the following mechanism based on the results shown above. Because Ti has the largest thermomigration force among Ti, Cu and Al, it can easily migrate under the present test condition. As soon as Ti in the second Ti layer diffuses into the Cu UBM, Al starts to migrate to the cold end to form Al–Cu solid solution or Al–Cu IMCs, resulting in void formation inside the Al trace. Under the present test condition, thermomigration of Cu also occurs in solder joints [13]. However, the thermomigration of Ti appears faster than that of Cu. As soon as the Ti layer is destroyed, Al atoms diffuse into the Cu UBM, resulting in the void formation in the Al trace. As shown in Figure 2b, the voids in the Al trace appear larger than those in the Cu–Sn IMCs. Therefore, Ti thermomigration might be the main reason accounting for the void formation inside the Al trace.

In summary, a high level of thermomigration of Ti is observed in flip-chip solder joints. When a thermal gradient is established across the Ti layer between the Al trace and the Cu UBM, Ti atoms are susceptible to migrate to the cold end because Ti possesses a very large heat of transport value of -768 kJ mol^{-2}. Once the Ti layer is damaged, Al atoms can easily diffuse into the Cu UBM to form Cu–Sn IMCs, leaving voids behind in the Al trace.

The financial support from the National Science Council, Taiwan, under the contract NSC 98-2221-E-009-036-MY3, is acknowledged.

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.scriptamat.2012.01.020.

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