SCIENTIFIC REPORTS

OPEN

A new failure mechanism of electromigration by surface diffusion of Sn on Ni and Cu metallization in microbumps

Yuan-Wei Chang¹, Chia-chia Hu¹, Hsin-Ying Peng¹, Yu-Chun Liang¹, Chih Chen¹, Tao-chih Chang², Chau-Jie Zhan² & Jing-Ye Juang²

Microbumps in three-dimensional integrated circuit now becomes essential technology to reach higher packaging density. However, the small volume of microbumps dramatically changes the characteristics from the flip-chip (FC) solder joints. For a 20 μm diameter microbump, the cross-section area and the volume are only 1/25 and 1/125 of a 100 μm diameter FC joint. The small area significantly enlarges the current density although the current crowding effect was reduced at the same time. The small volume of solder can be fully transformed into the intermetallic compounds (IMCs) very easily, and the IMCs are usually stronger under electromigration (EM). These result in the thoroughly change of the EM failure mechanism in microbumps. In this study, microbumps with two different diameter and flip-chip joints were EM tested. A new failure mechanism was found obviously in microbumps, which is the surface diffusion of Sn. Under EM testing, Sn atoms tend to migrate along the surface to the circumference of Ni and Cu metallization to form Ni_3Sn_4 and Cu_3Sn IMCs respectively. When the Sn diffuses away, necking or serious void formation occurs in the solder, which weakens the electrical and mechanical properties of the microbumps. Theoretic calculation indicates that this failure mode will become even significantly for the microbumps with smaller dimensions than the 18 μm microbumps.

Microbumps in three-dimensional integrated circuit (3D-IC) have emerged as a critical technology for the demand of better performance and higher packaging density^{1–4}. Since the shrinkage of Si devices does not catch up with the Moore's law, the 3D-IC technology provides an alternative way to maintain the increasing rate of packaging density^{2,4,5}. Microbumps have been adopted as interconnects between chips, and they are fabricated through a transient liquid phase reaction. However, the contact area of a microbump is only 1/25 of a flip-chip (FC) bump. With the reduction of contact area, the current density flowing in a microbump becomes much larger than that in a conventional FC bump. For a 20 μm microbump applied by 0.2 A, the current density reaches $6.37 \times 10^4 \text{ A/cm}^2$, which is far above the threshold value of Sn electromigration (EM)^{6–8}. Furthermore, the volume of a microbump is smaller than that of a FC bump by two orders, which may differ the EM failure mechanism in microbumps from the reported mechanisms in FC bumps. There were two main EM failure mechanisms reported^{9,10}: the void propagation along the IMC/solder interface^{11–14} and the dissolution of under-bump-metallization (UBM)^{15–20}. Both of them were correlated with the current crowding effect in the FC bumps. The small amount of solder in microbumps did not only reduce the current crowding effect^{21,22}, it also could be fully transformed into the IMC in a short time. These characteristics significantly elongated the EM failure and caused the microbumps immortal in some specific test conditions^{23–25}. Therefore, it is important to understand the EM failure mechanism inside microbumps. Some researchers have reported that surface diffusion of Sn occurred in microbumps during transient liquid phase reactions^{26,27}. This is a very important phenomenon because the surface diffusion of Sn on Ni or Cu is much faster than the grain boundary (GB) diffusion and the lattice diffusion. Bokshteyn *et al.* reported the surface diffusion of Sn on Ni was 8 and 10 orders faster than the GB diffusion and the lattice diffusion at high temperature (700 °C)^{28,29}. Besides, the diffusion was significantly enhanced by the EM³⁰. However, there is

¹Department of Materials Science and Engineering, National Chiao Tung University, Hsin-chu, 30010, Taiwan, Republic of China. ²Electronic and Optoelectronic System Research Laboratories, Industrial Technology Research Institute, Hsin-chu, Taiwan, 31040, Republic of China. Correspondence and requests for materials should be addressed to Y.-W.C. (email: aone.chang@gmail.com) or C.C. (email: chih@mail.nctu.edu.tw)

Figure 1. (a) The SEM image of the as-fabricated 18 μm microbump; The SEM image showing (b) the UBM dissolution and (c) the void formation induced by EM after 9.2×10^4 A/cm² at 150 °C for 192.3 and 50.0 h, respectively; The resistance increase due to (d) the UBM dissolution in (b), and (e) the void formation in (c).

no study yet to investigate EM failure in solder state in microbumps caused by the surface diffusion of Sn on the circumference of Ni and Cu UBMs. In this study, we applied EM testing on microbumps with different diameters and FC bumps. All of the UBM in these tested samples were Cu 5 μm/Ni 3 μm. Then a new EM failure mechanism, the surface diffusion of Sn, was found in microbumps with small volume of solder.

Results

An as-fabricated 18 μm-diameter microbump was shown in Fig. 1(a). It showed a very important specialty of microbump. The volume of solder became very small and inferior to the volume of UBM significantly. In this case, the solder could be fully consumed and transformed into IMC in a short time, as shown in Fig. 1(b). Figure 1(b and c) showed the microbumps EM tested by 9.2×10^4 A/cm² at 150 °C for 192.3 and 50.0 h respectively. The IMCs including Ni₃Sn₄, Cu₆Sn₅, and Cu₃Sn were found with much better EM resistance than the solder according to the higher critical product. The critical product indicates the ability of materials to resist EM, and it is represented as³¹

$$C. P. = L_c j_c = \frac{\sigma_c \Omega}{Z^* e \rho} \quad (1)$$

where L_c is the critical length, j_c is the critical current density, σ_c is the stress as the critical length, Ω is the atomic volume, Z^* is the effective charge number, e is the charge of electron, and ρ is the resistivity. If we take the stress at the elastic limit, the stress is the yield strength, σ_y . From the parameters in Table 1, we could not find big difference between Ω , Z^* , and ρ . However, the σ_c of IMCs are at 45 to 57 times higher than that of solder. Accordingly, the EM resistance of all IMCs are much higher than that of solder as well. Once solder reacts with the UBM and

Material	σ_y	Density (g/cm ³)	M_{avg} (g/mol)	Ω (10 ⁻²³ cm ³)	Z^*	ρ ($\mu\Omega$ -cm)
Sn3.5Ag	24.8 MPa ^{50,51}	7.4 ³³	118.69	2.66 2.705 (Sn) ⁵² 2.7 (Sn) ⁵³ 2.72 (Sn) ⁵⁴	18 ³⁰	12.3 ⁵⁵ 12.32 ⁵⁰
Cu ₆ Sn ₅	1.15 GPa ⁵¹	8.28 ⁵⁰	88.62	1.78 2.0 ¹⁸	68–87 ⁵⁶ 50 ¹⁸ 26 (Cu) ⁵⁷ 36 (Sn) ⁵⁷	17.54 ⁵⁰
Cu ₃ Sn	1.41 GPa ⁵¹	8.90 ⁵⁰	77.34	1.44	27 (Cu) ⁵⁷ 24 (Sn) ⁵⁷	8.93 ⁵⁰
Ni ₃ Sn ₄	1.13 GPa ⁵¹	8.65 ⁵⁰	92.98	1.79	21 (Ni) ⁵⁴ 21 (Sn) ⁵⁴	28.57 ⁵⁰

Table 1. The parameters for the calculation of the critical product. M_{avg} : Average atomic weight; $\Omega = \text{Density}/M_{avg}$.

fully transforms into IMCs, the microbump becomes an IMC joint, which can sustain under EM for a long time. That tremendously change the EM failure mechanism in microbumps rather than FC bumps.

In the previous studies of FC bumps, there were two EM failure mechanisms reported: (1) the void propagation along the IMC/solder interface^{11–14,32} and (2) the fast UBM dissolution/IMC formation^{15–20,33–35}. Due to the small volume of solder in microbump, the fast reaction between UBM and solder no longer caused the joint failure. Instead, the formation of IMC joint significantly elongated the EM failure time²³. Moreover, the fast IMC formation suspended the void propagation as shown in Fig. 1(c). Sometimes the fast transformation was accompanied by the void formation at the IMC/solder interface. However, the volume of solder was too small, and the height of solder was too short. The full transformation from solder into IMCs was faster than the void propagation through the entire interface so the void propagation was stopped. The formation of IMC joint overtook the effect of void propagation in this case. The microbump resistances of full transformation and void propagation, shown in Fig. 1(d and e) respectively, indicates the same tendency. The full transformation from the solder into IMC (in Fig. 1(b)) induced only 4.46 m Ω of resistance increase, which was 3.72% of the total microbump resistance (119.77 m Ω). The void propagation was overtaken by the IMC formation and therefore did not cause obvious resistance increase as the void propagation in FC bumps did. Even we could already observe the discontinuous void at the entire interface, the consequent resistance increase was only 0.86 m Ω . However, a new EM failure mechanism, surface diffusion of Sn, was found in this study. It is a phenomenon that a big portion of Sn diffused along the circumference surface of UBM and then induced the open failure.

Comparing with the as-prepared microbump shown in Fig. 1(a), surface diffusion of Sn occurs on the circumference of the Ni/Cu UBM during the current stressing in microbumps. Figure 2(a) showed a dummy microbump suffered from the same thermal history as the current stressed microbump in Fig. 2(c). There was still 2.7 μm -thick solder remained un-reacted, and the surface diffusion of Sn was not obvious in the dummy microbump without current stressing. Instead, it was significantly activated by the current stressing in the EM tested microbumps (Fig. 2(b and c)). The surface diffusion drains Sn atoms to the circumference and causes the serious void formation and necking in microbumps. Figure 2(b) presents the cross-sectional SEM image of the microbump after EM tested under $9.2 \times 10^4 \text{ A/cm}^2$ at 150 °C. We could observe the beginning of the surface diffusion of Sn at the circumference of the anode UBM (marked by the dashed rectangles). There were still some solder unreacted, and an obvious void was already able to be observed. The corresponding resistance (Fig. 2(d)) showed a different behavior from the resistance curves of UBM dissolution and void propagation. The resistance gradually increased in the beginning of EM testing. The growth of IMC was responsible for the lifting of microbump resistance. While the side-diffusion induced the void formation, the resistance increase immediately reacted by raising from 1.35 to 3.29 m Ω in 7.94 h. Figure 2(c) presents the cross-sectional SEM image for the microbump after the upward current stressing at $9.2 \times 10^4 \text{ A/cm}^2$ for 143 h. The corresponding resistance was demonstrated in Fig. 2(e). Serious void formation was observed in this microbump. Almost all the solder were transformed into Ni₃Sn₄ intermetallic compounds (IMCs). It is noteworthy that significant amount of Sn diffused to the circumference of the top UBM and formed Ni₃Sn₄ and Cu₃Sn IMCs there, as labeled by the dashed rectangles in the figure. On the contrary, the dummy microbump did not have obvious surface diffusion of Sn, and there was still 2.7 μm -thick solder remained unreacted. Unlike the slight increase of microbump resistance induced by the UBM dissolution and void propagation, the serious void formation induced by the surface diffusion of Sn caused several hundred milli-ohm of resistance increase as shown in Fig. 2(e). Besides, the microbump resistance in the late stage of EM testing was very unstable.

The surface diffusion of Sn in microbumps was a very common phenomenon; it did not only happen in the extreme testing conditions. Due to the chip-on-chip (COC) package, the heat dissipation of the tested samples were very good. Figure 3(a and c) demonstrated the cross-sectional temperature distribution in a stressing microbump and the temperature increase obtained by the simulation and the infrared microscope (IR). A $8.0 \times 10^4 \text{ A/cm}^2$ current density only induced 3 °C of temperature increase as shown in Fig. 3(c). Even a $9.2 \times 10^4 \text{ A/cm}^2$ current density barely induced 5 °C of temperature increase in the solder. The ambient temperature of EM testing was 150 °C. With the temperature increase induced by Joule heating, the maximum temperature of solder in the EM testing microbump did not exceed 155 °C, which should not significantly affect the failure mechanism. The cross-sectional current density distribution in the current stressing microbump was shown in Fig. 3(b). Because of the small diameter of microbumps, the difference of cross-section area between the traces and the microbumps was not big. Therefore, the current crowding effect is very slight in the microbumps^{21,22}. As shown in Fig. 3(b), the maximum current density was only $4.80 \times 10^4 \text{ A/cm}^2$ when the average one was $4.66 \times 10^4 \text{ A/cm}^2$. However, the necessary conditions to activate the surface diffusion of Sn were still not clear. The surface diffusion of Sn

Figure 2. (a) The SEM images of the dummy 18- μm microbump suffered from the same thermal history as the current stressed bumps. Only IMC thickening was observed. After EM tested under $9.2 \times 10^4 \text{ A/cm}^2$ at 150°C , side diffusion took place in microbumps. (b) With slight side-diffusion of Sn and (c) With severe void formation and failure caused by side-diffusion Sn; (d) The resistance curve for the microbump in (b), and (e) The resistance for the microbump in (c), which indicates the failure under EM testing.

occurred on the circumference of both the cathode and anode UBM. The present observation only implies that the EM is an important activation because the surface diffusion of Sn was not found in most of the dummy microbumps. More study is required on this topics.

The surface diffusion of Sn appears to be a universal EM reliability issues, and similar phenomena occurred in the microbumps with $30 \mu\text{m}$ in diameter. Figure 4(a) presents the cross-sectional SEM image for the $30 \mu\text{m}$ microbump before EM tests. The UBM structure was $5 \mu\text{m-Cu}/2 \mu\text{m-Ni}$ and the solder height approximately $5.7 \mu\text{m}$. Daisy chain structures of 40 microbumps were adopted for EM tests. After current stressing by $4.0 \times 10^4 \text{ A/cm}^2$ at 150°C for 2320 h, severe void formation occurred in some of the microbumps. Figure 4(b) presents the worst microbump with almost open failure. The electrons drifted downward in this bump. All the SnAg solders between the top and between UBMs were transformed into Ni_3Sn_4 IMC. The surface diffusion of Sn took place in both top and the bottom circumference of the Cu UBMs. The Sn atoms also reacted with the Ni and Cu to form Ni_3Sn_4 and Cu_3Sn IMCs, respectively. This is because there was more Cu than Sn on the side wall of the Cu UBM. Therefore Cu_3Sn formed instead of Cu_6Sn_5 IMCs. Diffusion of Sn on the circumference of Ni and Cu also occurred in other microbumps in the daisy chains. Figure 4(c) present another microbump having the surface diffusion of Sn and serious void formation. The microbump in Fig. 4(c) had the surface diffusion of Sn on both the top and bottom Cu UBMs. Serious necking was observed on the right side of the microbumps. On the contrary, the surface diffusion was not found in the dummy microbump in Fig. 4(d). Although some voids were also observed in the dummy microbump, it was obvious the microbump became an IMC bump and lasted for longer. The open failure caused by big voids (Fig. 4(b)) and the necking of joint (Fig. 4(c)) could not be found in the dummy microbumps.

Figure 3. The simulated (a) distribution of temperature and (b) distribution of current density in the 18 μm microbump; (c) Plot of solder temperature against applied current density obtained from the simulation and infrared microscopy (IR).

Actually, the surface diffusion of Sn (solder) induced by EM could also be found in the 120 μm-diameter FC solder joint as shown in Fig. 5. The dashed rectangles in Fig. 5 indicated the UBM circumference of FC joints. The dummy joints in Fig. 5(a) suffered from the same thermal history as the current stressing joints, and no surface diffusion of Sn was found in the dummy ones. On the contrary, the surface diffusion of Sn were significant in both of the FC joints tested by the upward and downward electron flow as shown in Fig. 5(b and c) respectively. However, the failure was mainly caused by the void propagation along the IMC/solder interface. The surface diffusion of Sn did not play an important role in the EM failure mechanism in the FC solder joints. As a result, it is very obvious that the small volume of Sn (solder) emphasized the importance of surface diffusion effect.

Discussion

The surface diffusion of Sn emerges to be the main EM failure mechanism in microbumps in this study. This is because the solder volume is very small, and once some solders are drawn away, voids form in the microbumps. Interestingly, the surface diffusion of Sn was only observed in current stressed microbumps and flip-chip joints as shown in Figs 2, 4, and 5. Sometimes the surface diffusion was only found at the anode side (Fig. 2(b and c)); sometimes it was found at both of the anode and cathode side. Because the metal atoms was driven by the electronic wind force during the EM testing³¹, it is reasonable that the surface diffusion appeared at the anode side. The surface diffusion at cathode side might be induced by the back stress in the solder generated by electron flow³⁶. The electron flow drove atom from cathode end to the anode end, and the back stress would increase the stress in the solders and try to push the Sn atoms back to cathode. It is speculated that at some locations in the cathode end of solders, the stress may be high enough to trigger the Sn atoms in the periphery of the microbumps to move to the side walls of the UBMs. Therefore, we occasionally observed side diffusion in the cathode end. Taking Ni for example, the surface diffusion coefficient is higher than the bulk and grain boundary diffusion by 10 and 8 orders at 700 °C^{28,29}. No matter of the surface diffusion at the anode or cathode side, current stressing was the most important factor that triggered the surface diffusion. The surface diffusion of Sn was only observed in the current stressed microbump or flip-chip joints.

In the following paragraphs, we will calculate the volume of Sn diffusion to the side walls of Ni and Cu UBMs. In the microbump in Fig. 2(c), the average thickness of the voids was measured to be 2.0 μm. The diameter of the microbump is 18 μm, so the volume of the voids was estimated to be 514.0 μm³. On the other hand, the original volume of the solder was calculated to be 1577.0 μm³. It is noteworthy that the formation of Ni₃Sn₄ IMCs induces 10.7 and 7.1% of volume shrinkage when the Ni₃Sn₄ and Cu₃Sn are forming, as depicted in Table 2. The volume shrinkage may cause voids with volume of 168.8 μm³ (=1577 μm³ × 10.7%) if the solder is fully reacted into Ni₃Sn₄. Therefore, approximate Sn volume of 345.2 μm³ (=514–168.8 μm³) was induced by the surface diffusion of Sn to the circumference of the Cu and Ni UBMs.

Figure 4. (a) The SEM image of the as-prepared microbump with $30\mu\text{m}$ in diameter; (b) and (c) the SEM image of microbumps showing severe void formation or necking after the EM test by $4.0 \times 10^4\text{ A/cm}^2$ at 150°C for 2320 h; (d) the SEM image of the dummy microbump with the same thermal history as the stressed microbumps.

We will calculate the depleted solder volume due to the surface diffusion of Sn using Fig. 2(c). As indicated in the figure, Sn atoms diffused to the circumference of the top Ni and Cu UBMs, and they reacted with Ni and Cu to form Ni_3Sn_4 and Cu_3Sn , respectively. The thickness of the Ni_3Sn_4 and Cu_3Sn was measured to be $1.5\mu\text{m}$ and $1.5\mu\text{m}$, respectively. The height of the Ni_3Sn_4 and Cu_3Sn was $2.5\mu\text{m}$ and $4.0\mu\text{m}$, respectively. We assumed the thickness of the Ni_3Sn_4 is the same of every location of the circumference of the Ni UBM, and the thickness of the Cu_3Sn is also the same at everywhere of the periphery of the Cu UBM. The consumed volume of Sn can be calculated using the volume ratio of Ni_3Sn_4 and Cu_3Sn in Table 2. The Sn volume consumed by the Ni_3Sn_4 and Cu_3Sn formation is $135.3\mu\text{m}^3$ and $186.3\mu\text{m}^3$, respectively. The sum of these two values yields $322.2\mu\text{m}^3$ ($=186.7 + 135.5\mu\text{m}^3$), which is close to the void volume of $345.2\mu\text{m}^3$ in the previous paragraph. Therefore, surface diffusion of Sn serves the main reason causing the void formation in the microbumps during the EM.

It is noteworthy that the Sn atoms also diffused to the circumference of the UBM in traditional FC solder joints as shown in Fig. 5(b and c)^{9,37–41}. However, no necking or void formation caused by the out diffusion of Sn atoms. This is because there are plenty of Sn in FC solder joints. For a typical FC joint with a diameter of $100\mu\text{m}$ and a bump height of $80\mu\text{m}$, the total solder volume was estimated to be $6.3 \times 10^5\mu\text{m}^3$ as shown in Table 3. If we assume the UBMs consists of $5\mu\text{m}$ Cu and $3\mu\text{m}$ Ni, and Sn atoms also diffuse to the side walls of Cu and Ni UBMs to form Cu_3Sn and Ni_3Sn_4 . The depleted Sn volume is $852.6\mu\text{m}^3$ and $1014.3\mu\text{m}^3$ due to the formation of Cu_3Sn and Ni_3Sn_4 respectively, resulting in only 0.3% of depletion of solder volume. Therefore, no necking or serious void formation due to the surface diffusion of Sn atoms. Nevertheless, the volume percentage of the surface diffusion increases as the dimension of the solder joint decreases. Table 3 lists the depletion percentage for the solder joints with $100\mu\text{m}$, $50\mu\text{m}$, $30\mu\text{m}$, $18\mu\text{m}$, and $12\mu\text{m}$. The calculation demonstrates that the depletion volume percentage is 0.3%, 1.6%, 7.8%, 20.4%, 46.3%, respectively. Figure 6 presents the percentage of Sn consumed by the surface diffusion as a function of the diameter of the UBM. The calculation assume the UBM is $5\mu\text{m}$ -thick Cu/ $3\mu\text{m}$ -thick Ni for all the solder joints in Table 3. It is noted that the thickness of the UBM cannot be reduced because of the reliability concern of metallurgical reactions. If the UBM is too thin, spalling of IMCs may occur

Figure 5. (a) The SEM image of the dummy 120- μm FC solder joints suffered from the same thermal history as the current-stressed joints. The SEM image showing the microstructure for the joint stressed by (b) an upward and (c) a downward electron flow for 1087 h.

Material	Molecular Weight (g/mol)	Density (g/cm ³)	Normalized volume (%)
Cu	63.6	8.96	56.9
Sn	118.76	7.37	43.1
Cu ₃ Sn	309.4	8.90	92.9
Ni	58.7	8.91	23.5
Sn	118.76	7.37	76.5
Ni ₃ Sn ₄	650.9	8.65	89.3

Table 2. The volume ratio during the following reactions: $3\text{Cu} + \text{Sn} \rightarrow \text{Cu}_3\text{Sn}$ and $3\text{Ni} + 4\text{Sn} \rightarrow \text{Ni}_3\text{Sn}_4$. The normalized volume is the volume of elements (compounds) normalized to the initial total volume.

D_{UBM} (μm)	h_{so} (μm)	V_{so} (μm^3)	V_{NS} (μm^3)	V_{so}^1 (μm^3)	V_{CS} (μm^3)	V_{so}^2 (μm^3)	V_{sd} (%)
12.0	4.0	4.5×10^2	147.3	126.2	179.1	83.1	46.3
18.0	6.2	1.6×10^3	217.9	186.7	292.2	135.5	20.4
30.0	10.0	7.1×10^3	359.3	307.8	518.4	240.5	7.8
50.0	30.0	5.9×10^4	594.9	509.7	895.4	415.4	1.6
100.0	80.0	6.3×10^5	1184.0	1014.3	1837.8	852.6	0.3

Table 3. The volume percentage of solder depleted by surface diffusion of Sn. D_{UBM} : the diameter of UBM. h_{so} : the height of solder. V_{so} : the total volume of solder. V_{NS} : the volume of Ni₃Sn₄ on the circumference of Ni UBM. V_{so}^1 : the solder consumed by the Ni₃Sn₄. $V_{\text{so}}^1 = V_{\text{NS}} \times 76.5/89.3$. V_{CS} : the volume of Cu₃Sn on the circumference of Cu UBM. V_{so}^2 : the solder consumed by the Cu₃Sn. $V_{\text{so}}^2 = V_{\text{CS}} \times 43.1/92.9$. V_{sd} : the solder consumed by the surface diffusion. $V_{\text{sd}} = (V_{\text{so}}^1 + V_{\text{so}}^2)/V_{\text{so}}$.

during reflow^{12,42–45}. Or the UBM will dissolve completely in the beginning stage of EM testing^{46,47}. In the present study, the out diffusion of Sn atoms depletes 20.4% ($322.2\mu\text{m}^3$) of the solder in the microbumps with $18\mu\text{m}$ in diameter. As the dimension shrinks down to $12\mu\text{m}$ in diameter, the surface diffusion of Sn will deplete 46.3% of the solder in the microbumps. Therefore, surface diffusion of Sn will be a critical issue for EM in microbumps, and it may dominate the failure mode of EM.

By the surface diffusion shown in Fig. 2(c), a minimum diffusion coefficient was obtainable. The diffusion length from the geometric center of depleted Sn to the circumference is $13\mu\text{m}$, and the diffusion took 53.5 h to achieve (the timing that the resistance suddenly raised). The diffusion velocity equals $13\mu\text{m}/53.5\text{ h}$, and that is $6.75 \times 10^{-9}\text{ cm/s}$. The diffusion flux, J , can be represented as:

Figure 6. The volume percentage of depleted solder due to the surface diffusion of Sn as a function of UBM diameter.

$$J = Cv \quad (2)$$

where C is the concentration and v is the diffusion velocity. The flux induced by EM, J_{EM} , is³¹

$$J_{em} = C \frac{D}{kT} Z^* e \rho j \quad (3)$$

where D is the diffusion coefficient, k is Boltzmann's constant, T is the temperature, Z^* is the effective charge number, e is the electron charge, ρ is the resistivity, and j is the applied current density. By combining Eq. 2 and Eq. 3, we obtain

$$D = \frac{vkT}{Z^* e \rho j} \quad (4)$$

Considering the Joule heating, the temperature of Sn was 155 °C (428 K) under 9.2×10^4 A/cm² of current stressing. According to previous study, Z^* of Sn is 17⁴⁸. The resistivity, ρ , of Sn3.5Ag is 12.5 μΩ-cm. Therefore, the diffusion coefficient, D , was calculated as 1.27×10^{-11} cm²/s. In this calculation, the v was underestimated because the sudden resistance change could only detect the timing of void formation induced by surface diffusion. However, the beginning of surface diffusion was not achievable. To obtain the diffusion velocity, we took the beginning of EM testing as the beginning of surface diffusion. It is highly possible for us to overestimate the total time of surface diffusion and therefore underestimate the diffusion velocity and the diffusion coefficient as well. In previous study, the diffusion coefficient of Sn to diffuse in Ni was 2.65×10^{-12} and 3.73×10^{-12} cm²/s at 160 and 180 °C⁴⁹. The self diffusion coefficient was 4.7×10^{-15} cm²/s at 150 °C³². The value we obtained by surface diffusion was higher than the values in previous study by 1 to 3 orders, which agreed with the previous study^{28,29}. The fast surface diffusion of Sn caused a new EM failure mechanism, which may be more important than the UBM dissolution and void propagation in the microbumps with tiny volume of solder.

Conclusions

In summary, we observed a new EM failure mechanism in microbumps, surface diffusion of Sn. Sn atoms diffused along the surface of the circumferences of the Ni and the Cu UBMs during EM testing, and formed Ni₃Sn₄ and Cu₃Sn, respectively. Unlike the slight resistance changes induced by UBM dissolution and void propagation, the void induced by the surface diffusion of Sn caused several hundred milli-ohm of resistance increase. Although the necessary condition to activate the surface diffusion of Sn was unclear, the EM was definitely a very important factor. Besides, the surface diffusion of Sn also happened in FC solder joints but did not play an important role because of the large solder volume. The small volume of Sn emphasized the importance of surface diffusion. The depletion percentage of the Sn volume was calculated to be approximately 20.4% of the original solder volume of the microbump with 18 μm in diameter. In addition, the depletion of the Sn caused serious void formation or necking in the microbumps, resulting in deteriorating electrical and mechanical properties. This failure mode will become even significantly for the microbumps with smaller dimensions than the 18 μm microbumps. According to our calculation, the surface diffusion coefficient of Sn should be higher than 1.27×10^{-11} cm²/s, which exceeded the value of Sn diffusion in Ni by several orders. Therefore, it is urgent to figure out the solution to the surface diffusion of Sn atoms onto the circumferences of the UBMs.

Methods

Microbumps of Sn2.5Ag with Cu/Ni UBM on both chip side and interposer side were selected for electromigration tests. Two kinds of microbump were adopted for EM tests: 18 μm and 30 μm diameter. The structures were vertically symmetric: the dimensions and materials of UBMs on the chip side and on the interposer side were the same. Figure 1(a) present the cross-sectional SEM image of the microbump with 18 μm in diameter before current

stressing. The thickness of Al pad was $0.8\text{ }\mu\text{m}$. The UBM was consisted of 100 nm thick Ti adhesive layer, $5.0\text{ }\mu\text{m}$ thick electroplated Cu, and $3.0\text{ }\mu\text{m}$ thick electroplated Ni. The Sn2.5Ag solder was made by electroplating, too. In the $18\text{ }\mu\text{m}$ microbump, the diameter of Al pad, passivation opening, and UBM opening were $20\text{ }\mu\text{m}$, $12\text{ }\mu\text{m}$, and $18\text{ }\mu\text{m}$ respectively. In the $30\text{ }\mu\text{m}$ microbump, they were $30\text{ }\mu\text{m}$, $18\text{ }\mu\text{m}$, and $30\text{ }\mu\text{m}$ respectively. The microbumps were bonded by thermo-compression at $280\text{ }^{\circ}\text{C}$ for a few seconds. After thermo-compression, the solder was $6.2\text{ }\mu\text{m}$ in height in the $18\text{ }\mu\text{m}$ microbump, and the Ni_3Sn_4 IMCs were about $1.0\text{ }\mu\text{m}$ thick on both the top and the bottom interfaces. Some dispersed Ag₃Sn particles were observed in the Sn2.5Ag solder. Yet the total thickness of the UBM layer was $16\text{ }\mu\text{m}$, thus the volume of the UBMs is larger than that of solder by 2.5 times. For traditional FC solder joints, the volume of solder is much larger than the volume of the UBMs as shown in Fig. 5. The diameter of passivation opening and UBM opening were 85 and $120\text{ }\mu\text{m}$ in the FC joints. This difference is expected to affect the EM behavior in the microbump significantly. The structure for the microbumps with $30\text{ }\mu\text{m}$ in diameter was shown in Fig. 4(a).

The applied current density in the $18\text{ }\mu\text{m}$ microbumps, the $30\text{ }\mu\text{m}$ microbumps, and the FC joints were 9.2×10^4 , 4.0×10^4 , and $7.1 \times 10^3\text{ A/cm}^2$. The EM tests were performed on a $150\text{ }^{\circ}\text{C}$ hotplate. After certain periods of EM testing, the current stressing was terminated and the tested samples were polished for microstructure analysis using a SEM. The $18\text{ }\mu\text{m}$ -diameter microbumps were also subjected to EM tests by $4.6 \times 10^4\text{ A/cm}^2$. However, we did not observe void formation due to the side diffusion of Sn in these microbumps. This may be attributed to the following reason: The length of trace in the $18\text{ }\mu\text{m}$ -microbump samples is shorter than that of the $30\text{ }\mu\text{m}$ -microbump samples. Therefore, the Joule heating effect induced $18\text{ }\mu\text{m}$ -diameter microbumps is lower, resulting no obvious EM effect at this stressing condition. The compositional simulation was performed by finite-element modeling.

References

1. Tu, K. Reliability challenges in 3d ic packaging technology. *Microelectronics Reliability* **51**, 517–523 (2011).
2. Chen, K.-N. & Tu, K.-N. Materials challenges in three-dimensional integrated circuits. *MRS Bulletin* **40**, 219–222 (2015).
3. Iyer, S. S. Three-dimensional integration: An industry perspective. *MRS Bulletin* **40**, 225–232 (2015).
4. Quinn, P. J. Silicon innovation exploiting moore scaling and “more than moore” technology. In *High-Performance AD and DA Converters, IC Design in Scaled Technologies, and Time-Domain Signal Processing*, 213–232 (Springer, 2015).
5. Patti, R. S. Three-dimensional integrated circuits and the future of system-on-chip designs. *Proceedings of the IEEE* **94**, 1214–1224 (2006).
6. Liu, C., Chih, C., Liao, C. & Tu, K. Microstructure-electromigration correlation in a thin stripe of eutectic snpb solder stressed between cu electrodes. *Applied Physics Letters* **75**, 58 (1999).
7. Choi, W., Yeh, E. & Tu, K. Mean-time-to-failure study of flip chip solder joints on cu/ni (v)/al thin-film under-bumpmetallization. *Journal of applied physics* **94**, 5665–5671 (2003).
8. Tu, K.-N. *Solder joint technology* (Springer, 2007).
9. Chen, C., Tong, H. & Tu, K. Electromigration and thermomigration in pb-free flip-chip solder joints. *Annual Review of Materials Research* **40**, 531–555 (2010).
10. Ke, J., Yang, T., Lai, Y. & Kao, C. Analysis and experimental verification of the competing degradation mechanisms for solder joints under electron current stressing. *Acta Materialia* **59**, 2462–2468 (2011).
11. Yeh, E. C., Choi, W., Tu, K., Elenius, P. & Balkan, H. Current-crowding-induced electromigration failure in flip chip solder joints. *Applied physics letters* **80**, 580–582 (2002).
12. Zeng, K. & Tu, K.-N. Six cases of reliability study of pb-free solder joints in electronic packaging technology. *Materials science and engineering: R: reports* **38**, 55–105 (2002).
13. Chang, Y., Liang, S. & Chen, C. Study of void formation due to electromigration in flip-chip solder joints using kelvin bump probes. *Applied physics letters* **89**, 032103 (2006).
14. Chang, Y., Chiang, T. & Chen, C. Effect of void propagation on bump resistance due to electromigration in flip-chip solder joints using kelvin structure. *Applied Physics Letters* **91**, 132113 (2007).
15. Gee, S., Kelkar, N., Huang, J. & Tu, K.-N. Lead-free and pbsn bump electromigration testing. In *ASME 2005 Pacific Rim Technical Conference and Exhibition on Integration and Packaging of MEMS, NEMS, and Electronic Systems collocated with the ASME 2005 Heat Transfer Summer Conference*, 1313–1321 (American Society of Mechanical Engineers, 2005).
16. Lin, Y., Tsai, C., Hu, Y., Lin, Y. & Kao, C. Electromigration-induced failure in flip-chip solder joints. *Journal of electronic materials* **34**, 27–33 (2005).
17. Lin, Y., Hu, Y., Tsai, C., Kao, C. & Tu, K. *In situ* observation of the void formation-and-propagation mechanism in solder joints under current-stressing. *Acta materialia* **53**, 2029–2035 (2005).
18. Zhang, L. *et al.* Effect of current crowding on void propagation at the interface between intermetallic compound and solder in flip chip solder joints. *Applied physics letters* **88**, 012106 (2006).
19. Chae, S.-H. *et al.* Electromigration lifetime statistics for pb-free solder joints with cu and ni ubm in plastic flip-chip packages. In *Electronic Components and Technology Conference, 2006. Proceedings. 56th*, 7–pp (IEEE, 2006).
20. Lee, J.-H. *et al.* Joule heating effect on the electromigration lifetimes and failure mechanisms of sn-3.5 ag solder bump. In *Electronic Components and Technology Conference, 2007. ECTC'07. Proceedings. 57th*, 1436–1441 (IEEE, 2007).
21. Kuan, W.-C., Liang, S. & Chen, C. Effect of bump size on current density and temperature distributions in flip-chip solder joints. *Microelectronics Reliability* **49**, 544–550 (2009).
22. Chang, Y. *et al.* Analysis of bump resistance and current distribution of ultra-fine-pitch microbumps. *Microelectronics Reliability* **53**, 41–46 (2013).
23. Ouyang, F.-Y., Hsu, H., Su, Y.-P. & Chang, T.-C. Electromigration induced failure on lead-free micro bumps in threedimensional integrated circuits packaging. *Journal of Applied Physics* **112**, 023505 (2012).
24. Chen, H.-Y. *et al.* Generic rules to achieve bump electromigration immortality for 3d ic integration. In *Electronic Components and Technology Conference (ECTC), 2013 IEEE 63rd*, 49–57 (IEEE, 2013).
25. Chen, H.-Y. *et al.* Electromigration immortality of purely intermetallic micro-bump for 3d integration. In *Electronic Components and Technology Conference (ECTC), 2015 IEEE 65th*, 620–625 (IEEE, 2015).
26. Liang, Y., Chen, C. & Tu, K. Side wall wetting induced void formation due to small solder volume in microbumps of ni/snag/ni upon reflow. *ECS Solid State Letters* **1**, P60–P62 (2012).
27. Panchenko, I. *et al.* Degradation of cu 6 sn 5 intermetallic compound by pore formation in solid-liquid interdiffusion cu/sn microbump interconnects. *Microelectronic Engineering* **117**, 26–34 (2014).
28. Boksteyn, S. Diffusion and the structure of metals. *Metal Science and Heat Treatment* **3**, 473–480 (1961).
29. Boksteyn, B. & Gubkova, T. Evaluation of the factors determining the change in diffusion mobility during deformation–ussr–. *Tech. Rep.*, DTIC Document (1960).

30. Chao, B. *et al.* Electromigration enhanced intermetallic growth and void formation in pb-free solder joints. *Journal of applied physics* **100**, 084909 (2006).
31. Tu, K.-N. Fundamentals of electromigration. In *Solder Joint Technology*, 211–243 (Springer, 2007).
32. Chao, B. *et al.* Investigation of diffusion and electromigration parameters for cu–sn intermetallic compounds in pb-free solders using simulated annealing. *Acta Materialia* **55**, 2805–2814 (2007).
33. Nah, J.-W., Kim, J. H., Lee, H. M. & Paik, K.-W. Electromigration in flip chip solder bump of 97pb–3sn/37pb–63sn combination structure. *Acta Materialia* **52**, 129–136 (2004).
34. Alam, M. O., Wu, B., Chan, Y. C. & Tu, K. High electric current density-induced interfacial reactions in micro ball grid array (μ bga) solder joints. *Acta materialia* **54**, 613–621 (2006).
35. Lu, Y.-D., He, X.-Q., En, Y.-F., Wang, X. & Zhuang, Z.-Q. Polarity effect of electromigration on intermetallic compound formation in snpb solder joints. *Acta Materialia* **57**, 2560–2566 (2009).
36. Chen, K. *et al.* “In situ measurement of electromigration-induced transient stress in Pb-free Sn–Cu solder joints by synchrotron radiation based x-ray polychromatic microdiffraction.” *Journal of Applied Physics* **106**(2), 023502 (2009).
37. Tsai, C., Lin, Y., Tsai, J., Lai, Y.-S. & Kao, C. Local melting induced by electromigration in flip-chip solder joints. *Journal of electronic materials* **35**, 1005–1009 (2006).
38. Lai, Y.-S., Chiu, Y.-T., Lee, C.-W., Shao, Y.-H. & Chen, J. Electromigration reliability and morphologies of cu pillar flip-chip solder joints. In *Electronic Components and Technology Conference, 2008. ECTC 2008. 58th*, 330–335 (IEEE, 2008).
39. Ha, S.-S., Kim, J.-W., Yoon, J.-W., Ha, S.-O. & Jung, S.-B. Electromigration behavior in sn-37pb and sn-3.0 ag-0.5 cu flip-chip solder joints under high current density. *Journal of Electronic Materials* **38**, 70–77 (2009).
40. Wright, S. *et al.* Characterization of micro-bump c4 interconnects for si-carrier sop applications. In *Electronic Components and Technology Conference, 2006. Proceedings. 56th*, 8–pp (IEEE, 2006).
41. Yoo, J.-H. *et al.* Analysis of electromigration for cu pillar bump in flip chip package. In *Electronics Packaging Technology Conference (EPTC), 2010 12th*, 129–133 (IEEE, 2010).
42. Liu, A. A., Kim, H., Tu, K. & Totta, P. A. Spalling of cu₆sn₅ spheroids in the soldering reaction of eutectic snpb on cr/cu/au thin films. *Journal of Applied Physics* **80**, 2774–2780 (1996).
43. Kim, H., Tu, K. & Totta, P. Ripening-assisted asymmetric spalling of cu–sn compound spheroids in solder joints on si wafers. *Applied Physics Letters* **68**, 2204–2206 (1996).
44. Tu, K.-N. & Zeng, K. Tin–lead (snpb) solder reaction in flip chip technology. *Materials science and engineering: R: reports* **34**, 1–58 (2001).
45. Tu, K. Recent advances on electromigration in very-large-scale-integration of interconnects. *Journal of applied physics* **94**, 5451–5473 (2003).
46. Chen, H.-Y. & Chen, C. Thermomigration of cu–sn and ni–sn intermetallic compounds during electromigration in pb-free snag solder joints. *Journal of Materials Research* **26**, 983–991 (2011).
47. Chen, H.-Y. *et al.* Thermomigration of ti in flip-chip solder joints. *Scripta Materialia* **66**, 694–697 (2012).
48. Huntington, H. Electromigration in metals. *Diffusion in solids recent developments* 303–352 (1975).
49. Chen, C.-M. & Chen, S.-W. Electromigration effect upon the sn/ag and sn/ni interfacial reactions at various temperatures. *Acta materialia* **50**, 2461–2469 (2002).
50. Lee, C. C., Wang, P. J. & Kim, J. S. Are intermetallics in solder joints really brittle? In *Electronic Components and Technology Conference, 2007. ECTC'07. Proceedings. 57th*, 648–652 (IEEE, 2007).
51. Ghosh, G. Elastic properties, hardness, and indentation fracture toughness of intermetallics relevant to electronic packaging. *Journal of materials research* **19**, 1439–1454 (2004).
52. King, H. & King, H. Atomic size parameters for the elements. *Journal of Phase Equilibria* **2**, 527–528 (1982).
53. Chen, L.-T. & Chen, C.-M. Electromigration study in the eutectic snbi solder joint on the ni/au metallization. *Journal of materials research* **21**, 962–969 (2006).
54. Wang, Y. & Ho, P. S. Mode ii electromigration failure mechanism in sn-based pb-free solder joints with ni under-bump metallization. *Applied Physics Letters* **103**, 121909 (2013).
55. Glazer, J. Metallurgy of low temperature pb-free solders for electronic assembly. *International Materials Reviews* **40**, 65–93 (1995).
56. Ou, S. & Tu, K. A study of electromigration in sn3. 5ag and sn3. 8ag0. 7cu solder lines. In *Electronic Components and Technology Conference, 2005. Proceedings. 55th*, 1445–1450 (IEEE, 2005).
57. Chao, B. H.-L., Zhang, X., Chae, S.-H. & Ho, P. S. Recent advances on kinetic analysis of electromigration enhanced intermetallic growth and damage formation in pb-free solder joints. *Microelectronics Reliability* **49**, 253–263 (2009).

Acknowledgements

We acknowledge the financial support received from the Ministry of Science and Technology of Taiwan under contracts 102-2221-E-009-040-MY3.

Author Contributions

Y.W. Chang, C.C. Hu, and Y.C. Liang conducted the experiments; Y.W. Chang and H.Y. Peng did the simulation; Y.W. Chang analyzed the results; Y.W. Chang, T.C. Chang, C.J. Zhan and J.Y. Juang designed and fabricated the samples; All authors reviewed the manuscript.

Additional Information

Competing Interests: The authors declare no competing interests.

Publisher's note: Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

Open Access This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons license, and indicate if changes were made. The images or other third party material in this article are included in the article's Creative Commons license, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons license and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this license, visit <http://creativecommons.org/licenses/by/4.0/>.