Mechanism of improved electromigration reliability using Fe-Ni UBM in wafer level package

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\textbf{A R T I C L E   I N F O}

Article history:
Received 21 February 2017
Received in revised form 22 April 2017
Accepted 27 April 2017
Available online 1 December 2017

Keywords:
Fe-Ni under bump metallization (UBM)
Intermetallic compounds (IMCs)
Electromigration (EM)
Diffusion
Vacancy formation

\textbf{A B S T R A C T}

Fe-Ni films with compositions of 73 wt\% of Ni and 45 wt\% of Ni were used as under bump metallization (UBM) in wafer level chip scale package, and their reliability was evaluated through electromigration (EM) test compared with commercial Cu UBM. For Sn3.8Ag0.7Cu (SAC)/Cu solder joints, voids had initiated at Cu cathode after 300 h and typical failures of depletion of Cu cathode and cracks were detected after 1000 h EM. While the SAC/Fe-Ni solder joints kept at a perfect condition without any failures after 1000 h EM. Moreover, the characteristic lifetime calculated by Weibull analysis for Fe-73Ni UBM (2121 h), Fe-45Ni UBM (2340 h) were both over three folds to Cu UBM’s (698 h). The failure modes for Fe-Ni solder joints varied with the different growth behavior of intermetallic compounds (IMCs), which can all be classified as the crack at the cathodic interface between solder and outer IMC layer. The atomic fluxes concerned cathode dissolution and crack initiation were analyzed. When Fe-Ni UBM was added, cathode dissolution was suppressed due to the low diffusivity of IMCs and opposite transferring direction to electron flow of Fe atoms. The smaller EM flux within solder material led a smaller vacancy flux in Fe-Ni solder joints, which can explain the delay of solder voids and cracks as well as the much longer lifetime under EM.

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1. Introduction

Solder joining technology is used in various packaging applications such as wafer level chip scale package (WLCSP) and its evolutions. With the trend of multi-functionlization and miniaturization, electronic devices might endure much high current density and operation temperature during service with the decrease in bump size. Under such high current density and operation temperature, diffusion of atoms can occur easily.

Hence, electromigration (EM) performance becomes more and more important as a reliability issue. For SnAgCu solder on traditional Cu under bump metallization (UBM), EM significantly enhances the cathode consumption and the initiation of cracks [1]. Therefore, new materials aimed at improving EM resistance are under development. One of the strategies is to develop new solders by adding minor elements [2], while the other is to propose some novel materials as UBM barrier layer [3,4]. For a superior UBM material, performances such as diffusion barrier, wettability and EM resistance should be considered. Fe-Ni alloys were identified as superior diffusion barrier layers at the interface between lead free solder and Cu for their extremely slow growth rate of intermetallic compounds (IMCs) during aging test [5,6]. Besides, the alloys also have enough wettability for interfacial reaction [7,8]. However, researchers still wonder the EM reliability of Fe-Ni UBMs before accepting the alloys for industry application, which has never been investigated according to our knowledge.

In this study, a series of EM tests were applied to the special designed WLCSP vehicle in order to evaluate the reliability performances of Fe-Ni UBMs under EM. Compared with the commercial Cu UBM, the microstructural evolution and failure behavior at the interface of solder joints were characterized in detail. Weibull analysis shows that Fe-Ni UBMs possessed much longer lifetime than Cu UBM. And the mechanism of superior EM resistance of Fe-Ni UBMs was discussed considering the diffusion and reaction of metal atoms under the coupling of thermal and current stressing.

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https://doi.org/10.1016/j.jmst.2017.11.046
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2. Experimental

2.1. Preparation of test vehicle

Firstly, two Fe-Ni UBMs as well as commercial Cu UBMs were electroplated on 8-in. patterned wafers. The two Fe-Ni UBMs with composition of 73wt%Ni and 45wt%Ni were denoted as Fe-73Ni and Fe-45Ni, respectively. Details of the electroplating process were reported elsewhere [9,10], and the thickness of all different UBMs was about 7.5μm. In addition, the lead free solder used here was Sn3.8Ag0.7Cu, which was mentioned as SAC for simplicity. Then, the chip was reflowed upon the Cu/OSP pad within the printed circuit board (PCB) substrate (20 mm × 20 mm × 0.8 mm). The peak temperature of the reflow process was 245°C, and the time above the eutectic temperature (217°C) was 67 s. The PCB substrate and test sketch map are shown in Fig. 1. Notably, 70-μm-thick Cu pad on PCB substrate was designed intentionally. On the one hand, Cu pad on PCB side can be used as a reference to observe the EM behavior of Fe-Ni UBMs. On the other hand, it prevents the early depletion of Cu material under current stressing for the sake of the lifetime statistic of Fe-Ni UBMs.

2.2. Electromigration test

To keep uniform ambient temperature and prevent oxidation, all the vehicles were immersed in an oil bath (40°C) and the direct-current (DC) was 1.2 × 10^4 A/cm^2 during the EM test. The electrical resistance and temperature of vehicles were monitored through an in situ recorder (HIOKI LR8400-21). Due to the Joule heat, the temperature of each vehicle was around 150°C.

As for lifetime calculation, fifteen vehicles for each kind of UBMs were tested until failure. For each vehicle, sixty solder joints were electified in series through the daisy chain design with the flip-chip solder joints between the chip and the PCB as shown in Fig. 1(b). Once the open circuit happened on one of the sixty solder joints, it was set as the failure criterion of that vehicle. Thus, lifetime of each vehicle would be the minimum value of the sixty solder joints, which also provided a much reliable model to analyze the lifetime of vehicles in application.

2.3. Microstructural characterization

The microstructural observation was conducted after 300 and 1000 h current stressing. Cross sections of different solder joints were prepared by the standard metallographic techniques, and then were observed with a ZEISS supra 55 scanning electron microscope (SEM). The characterization focused mostly on the SAC/UBM interface at the chip side. A pair of solder joints was observed at the same time, where cathode was always on the upper left and anode on the upper right as shown in Fig. 1(c). Also, the elemental mapping and point analysis of EDS (energy dispersive spectroscopy) were applied during the identification of IMCs. Moreover, all SEM images presented in the following section were backscattered electron image, which can provide information about the distribution of different elements. Hence it is useful to distinguish different IMCs. In order to get clear morphologies of the interfacial IMCs within Fe-Ni solder joints, the cross sectional solder joints were etched sometimes during the SEM observation. However, non-etched morphologies are shown in the following section to present the failures induced during the EM test.

3. Results

3.1. Microstructural evolution of solder joints during electromigration

3.1.1. Interfacial microstructures before current stressing

Microstructures of three different solder joints after reflow are displayed in Fig. 2(a–c). There is a 1.9-μm-thick scalloped Cu6Sn5 layer generated at the SAC/Cu interface. And a very thin Cu3Sn was formed initially at the interface between Cu and Cu6Sn5 as depicted by black arrowheads in Fig. 2(a). As for Fe-73Ni UBMs, both FeSn2 and (CuNi)6Sn5 were formed at the interface as shown in Fig. 2(b), where the FeSn2 layer next to the UBMs is indicated by black arrowheads. Previous TEM results showed the thickness of FeSn2 layer was about 250 nm [11]. The (CuNi)6Sn5 was rod-like grains with 3–5 μm in length dispersing within the solder material near the interface, which was distinctly different from the eutectic microstructure of SAC solder material. As for Fe-45Ni UBMs (Fig. 2(c)), only a 250-nm-thick FeSn2 layer formed at the interface. Notably, the Ag3Sn granules in white contrast were dispersing within the solder matrix initially. While during the interfacial reaction, the dimension of Ag3Sn might grow larger and can be wrapped within IMC layers. Since they have little effect on the interfacial evolution, we will ignore them in the following description and discussion.

For comparison, the interfacial images of three different solder joints after annealing at 150°C for 1000 h are shown in Fig. 2(d–f). At the SAC/Cu interface, Cu4Sn5 was thickened from 1.9 μm (after reflow in Fig. 2(a)) to 3.8 μm after 1000 h aging (Fig. 2(d)). A 3.3-μm-thick Cu3Sn layer was generated between Cu UBMs and Cu6Sn5 layer, accompanying with a large amount of Kirkendall voids within Cu3Sn as seen in Fig. 2(d). At SAC/Fe-73Ni interface (Fig. 2(e)), rod-like (CuNi)6Sn5 were interconnected into a continuous outer layer. Moreover, plenty of FeSn2 granules were also diffused into outer (CuNi)6Sn5 layer during long time aging, which forms a mixed layer composed of FeSn2 granules and (CuNi)6Sn5 net structure as separated from the FeSn2 layer and (CuNi)6Sn5 layer by black and
white arrowheads, respectively. The IMC growth rate at SAC/Fe-45Ni interface is the slowest in Fig. 2(f). Two continuous IMC layers were found, which were 0.9 μm FeSn2 layer and 1.3 μm (Cu,Ni)5Sn3 from top to bottom, whose interface is indicated by black arrowheads in Fig. 2(f). It is clear that SAC/Fe-Ni solder joints process a much slower IMC growth rate compared with SAC/Cu solder joints, which indicates an excellent barrier effect on thermal diffusion for Fe-Ni UBMs under high temperature aging.

3.1.2. Interfacial microstructures after 300h current stressing

Fig. 3 reveals the microstructures of three different solder joints after 300h EM test. The major difference between the anode and cathode comes from the direction of electron flow, which is indicated by the arrows with symbol e⁻ in Fig. 3. Both substrate dissolution and IMC accumulation prefer to initiate at the corner of an interface, where the current flows in and out, which results from the current crowding effect [12]. The locations where current crowding is the most serious are highlighted by circles and enlarged in the bottom figures.

Firstly, a pair of SAC/Cu solder joints is displayed in Fig. 3(a). Several voids were detected at the Cu UBM cathode (upper left circle), while IMC accumulation was observed at the anode on the upper right side. Moreover, massive atoms transportation induced a large amount of bulk Cu5Sn3 on the right side within the right solder joint. As enlarged in Fig. 3(b), a large solder void with diameter more than 5 μm was initiated at the interface between the solder material and IMC layer. Due to the massive transportation of atoms under EM, the thickness of IMCs at Cu UBM anode (5.9 μm in Fig. 3(c)) was more than twice larger than that at the cathode (2.1 μm in Fig. 3(b)), indicating an obvious polarity effect.

Secondly, for SAC/Fe-73Ni interface as presented in Fig. 3(d), no failure was detected within the solder joints, while a “V” shape IMC layer was floating within the solder material at both cathode and anode. As enlarged in Fig. 3(e), island shape (Cu,Ni)5Sn3 grains generated as an outer layer beneath FeSn2 while some isolated rod-like grains as indicated by the white arrowheads formed the floating “V” shape IMC layer. At the anode of Fig. 3(f), (Cu,Ni)5Sn3 with irregular...
shape was formed, which was probably induced by the coarsening and interconnecting of scalloped and rod-like grains.

The SAC/Fe-45Ni solder joints (Fig. 3(g)) also kept at a perfect condition after 300 h current stressing. Owing to the outstanding diffusion barrier effect of Fe-45Ni UBM [13] and the migration of Cu atoms under EM effect, no (Cu,Ni)6Sn5 IMC was formed at the Fe-45Ni UBM cathode. There is only a FeSn2 layer at the interface as indicated in Fig. 3(h). Whereas, island shape (Cu,Ni)6Sn5 generated as a result of the substantial supply for Cu atoms at the anode (Fig. 3(i)). Remarkably, under the coupling effect of both the thermal diffusion and EM, FeSn2 kept as a thin film below 0.5 μm at both cathode and anode upon the Fe-73Ni and Fe-45Ni UBMs, indicating a difficult process for FeSn2 to increase or degrade. This should be attributed to the low diffusivity of Fe at SAC/Fe-Ni interface, which will be discussed in discussion section.

3.1.3. Interfacial microstructures after 1000 h current stressing

As shown in Fig. 4, various changes on microstructures were observed after 1000 h current stressing. For SAC/Fe-45Ni solder joints (Fig. 4(a)), serrated dissolutions were observed. Cu cathode had already been depleted in some place, and only some serrated Cu UBM material was left in the enlarged area as shown in Fig. 4(b). The voids between solder and IMC layer accumulated and propagated into a crack. Due to the migration of Cu atom from the cathode towards anode, thicker IMCs but less Kirkendall voids were observed at the anode (Fig. 4(c)). These results are consistent with the description in the literature of EM test [14].

However, no failure signs were detected at the Fe-73Ni cathode on the chip side after 1000 h EM (Fig. 4(d)). In contrast, the Cu cathode on the PCB side on the lower right was seriously consumed into an irregular shape with the formation of voids, which demonstrated a superior EM resistance in cathode dissolution for Fe-73Ni UBM compared with the conventional Cu material. There are three IMC layers at both the cathode and the anode, and the interfaces of IMC layers were indicated by the arrowheads, respectively. At the cathode of Fig. 4(e), the first layer next to the UBM was FeSn2 with a thickness of about 400 nm. The second layer was a mixed layer (3.4 μm), which consisted of fine FeSn2 granules and (Cu,Ni)6Sn5 net structure. The third outer layer was floating (Cu,Ni)6Sn5 grains. According to our observation, the mixed layer and the floating (Cu,Ni)6Sn5 layer at the cathode would shrink or disappear in some solder joints due to the migration of atoms. At the anode of Fig. 4(f), from UBM to the solder side three layers were observed: FeSn2 layer, mixed layer as well as Cu6Sn5 layer. The thickness of the FeSn2 layer is about 400 nm, and the mixed layer is 7 μm in thickness. The IMC at the anode is much thinner than that at the cathode (3.4 μm in Fig. 4(e)) and that after 150 °C aging for 1000 h without current (3.8 μm in Fig. 2(e)). Furthermore, the mixed layer under aging condition seems to contain more FeSn2 granules. Since the thickness of FeSn2 depends upon the Fe flux at the interface under the interaction of thermal diffusion and EM effect, it was deduced that the diffusion of Fe atoms was accelerated at the anode but suppressed at the cathode under current stressing, whose mechanism will be described in the discussion section.

For precise identification, the EDS results for different IMCs are listed in Table 1, which were summarized from at least six locations for each IMC at the interface of solder joint. The elemental mapping in Fig. 5 confirms the mixed layer of (Cu,Ni)6Sn5 and FeSn2 granules at SAC/Fe-73Ni interface. In order to distinguish different IMCs, a stronger contrast was applied in the SEM images of Fig. 5 compared to Fig. 4. For the situation at the cathode (Fig. 5(a)), the granules in white contrast upon the thin FeSn2 layer are also rich in Fe element according to the mapping of Fe element in Fig. 5(b), which represents FeSn2 phase. While the contrast of Cu map (Fig. 5(c)) is complementary to Fe map, indicating the formation of Cu-Sn IMC. Combined with the EDS point analyses, the contrast of Ni and Sn map (Fig. 5(d and e)) demonstrates the formation of (Cu,Ni)6Sn5. The situation for Fe-73Ni anode is shown in Fig. 5(f), and its corresponding EDS mapping results are shown in Fig. 5(g–j). As shown in the EDS map of Fig. 5(g), FeSn2 granules are dispersing uniformly within the mixed layer. Notably, the interface between the mixed layer and the outer layer was also obvious in the Cu and Ni maps (Fig. 5(h and i)), implying a concentration gradient for Cu and Ni elements between these two layers. Combined with the results in Table 1, the middle layer contains (28–34) at.% of Cu, (13–17) at.% of Ni, (5–9) at.% of Fe and (44–47) at.% of Sn, which was denoted as a mixed layer of FeSn2 and (Cu,Ni)6Sn5. Whereas, outer layer at the anode was denoted as Cu6Sn5 since no Fe and Ni were detected within it.

No failure was found on the Fe-45Ni cathode after 1000 h EM test (Fig. 4(g)). There is only an 800 nm layer of FeSn2 at the cathode.
Table 1
Constituent of the IMC layers after 1000 h EM.

<table>
<thead>
<tr>
<th>IMC layers from UBMs to solder</th>
<th>Elements (at.%)</th>
<th>Cu</th>
<th>Ni</th>
<th>Fe</th>
<th>Sn</th>
<th>Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe-73Ni</td>
<td>First layer at both cathode and anode</td>
<td>0–1.8</td>
<td>0–6.1</td>
<td>22.5–30.6</td>
<td>61.4–77.6</td>
<td>FeSn2</td>
</tr>
<tr>
<td></td>
<td>Second layer at both cathode and anode</td>
<td>27.9–33.8</td>
<td>13.0–16.7</td>
<td>5.3–8.9</td>
<td>44.0–46.7</td>
<td>FeSn2+ (Cu,Ni)6Sn5</td>
</tr>
<tr>
<td></td>
<td>Third layer</td>
<td>cathode</td>
<td>anode</td>
<td>39.8–50.3</td>
<td>9.0–12.0</td>
<td>0–1.1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>54.1–59.1</td>
<td>0</td>
<td>0</td>
<td>40.9–46.3</td>
<td>Cu6Sn5</td>
</tr>
<tr>
<td>Fe-45Ni</td>
<td>First layer at both cathode and anode</td>
<td>0</td>
<td>5.8</td>
<td>31.6</td>
<td>62.6</td>
<td>FeSn2</td>
</tr>
<tr>
<td></td>
<td>Second layer at anode</td>
<td>29.1–38.7</td>
<td>8.4–11.1</td>
<td>9.5–14.3</td>
<td>43.4–45.9</td>
<td>FeSn2+ (Cu,Ni)6Sn5</td>
</tr>
<tr>
<td></td>
<td>Third layer at anode</td>
<td>50.9–54.8</td>
<td>0</td>
<td>0</td>
<td>45.2–49.1</td>
<td>Cu6Sn5</td>
</tr>
</tbody>
</table>

Fig. 5. EDS mapping results: (a) Fe-73Ni cathode with (b) Fe, (c) Cu, (d) Ni and (e) Sn maps at Fe-73Ni cathode, respectively; (f) Fe-73Ni anode with (g) Fe, (h) Cu, (i) Ni and (j) Sn maps at Fe-73Ni anode, respectively.

(Fe. 4(b)). While three IMC layers were formed at Fe-45Ni anode as shown in Fig. 4(i), which were FeSn2 layer (0.5 μm), FeSn2 and (Cu,Ni)6Sn5 mixed layer (4.5 μm) as well as Cu6Sn5 layer (>20 μm) from the UBM side to solder side. The corresponding EDS results are also listed in Table 1.

It was concluded that after 1000 h EM test, fast consumption of Cu UBM induced serrated dissolution or even cathode depletion at SAC/Cu solder joint, and solder voids accumulated and propagated to generate cracks at the same time. However, there were no solder voids and serrated dissolution within Fe-Ni UBM even after 1000 h current stressing. Therefore, Fe-Ni UBM s have better EM resistance, and can overcome the drawbacks of fast consumption and solder voiding of Cu UBM.

3.2. Failure mode of Fe-Ni solder joints after EM test

As mentioned above, fast consumption of Cu cathode and solder voiding led to the failure of SAC/Cu solder joints, which is consistent with previous reports [15,16]. Therefore, failure mode was focused on and investigated in detail during the observation of the failed SAC/Fe-Ni solder joints, using conventional Cu UBM as a reference. In this work, EM test was conducted continuously until the open circle of the test vehicles happened. And solder joints with cracks longer than 5 μm in length during the microstructural observation were defined as a failure, and more than thirty pairs of failed solder joints were observed for each kind of UBM. It was found that all the failures happened at the cathode side of the SAC/Fe-Ni solder joints, which can be divided into two kinds of failure modes.

The microstructures of the failed Fe-Ni solder joints are displayed in Fig. 6. As for Fe-73Ni UBM, the exact location of cracks at the cathode varied with the different growth of IMCs, which can be categorized into two modes. In the first mode (Mode I), cracks initiated at the interface of IMC/solder near UBM. Fig. 6(a) shows a typical failure belong to Mode I, which was observed in a Fe-73Ni solder joint after 1649 h EM test. Three IMCs were observed at the cathode, which were FeSn2, (Ni,Cu)3Sn4 and (Cu,Ni)6Sn5 as shown in Fig. 6(b). The appearance of (Ni,Cu)3Sn4 was usually accompanied with the disappearance of mixed layer. So it was supposed that (Cu,Ni)6Sn5 within the mixed layer would transform into (Ni,Cu)3Sn4 as a result of the depletion of Cu element at the cathode during the EM test [17]. As shown in Fig. 6(b), (Cu,Ni)6Sn5 was almost consumed and only some grains were left beneath (Ni,Cu)3Sn4 layer. Moreover, the FeSn2 phase had processed into a 2-μm-thick layer instead of dispersing within the mixed layer compared with the situation of 1000 h EM test (Fig. 4(e)). In some failed solder joints within this kind of failure mode, only one or two IMC layers were left at the cathode. For example, there was only FeSn2 layer at the interface, and the (Cu,Ni)6Sn5 layer was totally dissolved before transforming into (Ni,Cu)3Sn4. Also occasionally, there were FeSn2 and (Ni,Cu)3Sn4 IMC layers at the interface, while the (Cu,Ni)6Sn5 had already been depleted. In addition, the IMCs at the anode are displayed in Fig. 6(c), which were FeSn2, FeSn2+ (Cu,Ni)6Sn5 mixed layer as well as Cu6Sn5 layers. Comparing Fig. 6(b and c), the differences of IMCs between cathode and anode were obvious. Large amount of Cu6Sn5 was accumulated at the anode while the (Ni,Cu)3Sn4 phase did not form. This can also
be explained by the atomic fluxes within solder joint too. Since Cu atoms transferred from PCB substrate towards the Fe-73Ni UBM anode as electron flows, the sufficient supply of Cu atoms at the anode is beneficial to the formation of (Cu,Ni)3Sn4 and (Cu,Ni)2Sn5 but not (Ni,Cu)3Sn4 phase.

In the second mode of Fe-73Ni solder joints, a V-shape IMC layer was formed within the solder, and cracks initiated at the interface of V-shape IMC/solder. Typical morphologies of a failed Fe-Ni solder joints after 2213 h EM test in this mode (Mode II) is revealed in Fig. 6(d). A part of IMC had spalled as an isolated layer and drifted into the solder, which results in the contrast of a “V” shape. The crack initiated and propagated at the outer side of the drifting IMCs. According to the observation, the drifted IMC layer was composed of (Cu,Ni)2Sn5 and (Ni,Cu)3Sn4 as shows in Fig. 6(e), which probably originated from the floating IMCs as described above in Fig. 3(d–f). At the initiation stage of EM test (300 h), there was a “V” shape IMC layer floating within the solder material, which was composed of tens of isolated rod like (Cu,Ni)2Sn5 grains. It was reported that the diffusion coefficient of Cu in IMC phase was about $5 \times 10^{-4}$ folds less than that in Sn phase [18]. So, if the floating IMCs interconnected with each other and formed a continuous layer, both the forwards and backwards atomic fluxes would be obstructed here. What’s more, solder voids induced by the vacancy flux were also congregate beyond this layer too. However, the second failure mode only took 16.7%, which is an unusual mode in the thirty failures of Fe-73Ni cathodes compared to the first mode. It was mainly because the floating rod like (Cu,Ni)2Sn5 grains were usually dissolved into the solder as the time increased, instead of forming the drifting IMC layer, so the electromigration-induced failure would mainly follow the first mode. Notably, the second failure mode happened merely in Fe-73Ni cathode, which also indicated that higher Fe content had a suppression effect on the drifting IMC under this situation. The IMCs at the anode in the second mode (Fig. 6(f)) was similar to those in the first mode (Fig. 6(c)).

Above all, the microstructural evolution at the Fe-73Ni cathode can be explained by the following process. At the initial stage, since the IMC layer is thin, the diffusion-driven chemical potential is large. Therefore, the IMC evolution acts the same as aging condition, and both FeSn2 and (Cu,Ni)2Sn5 form and grow thicker. After the IMCs become thick enough, the chemical potential decreases while the driving force of EM becomes prominent. The Cu and Ni atoms within solder material near IMC are migrating towards the anode under current stressing, resulting in an unsaturated concentration at the cathode. The concentration gradient between the IMC and nearby solder material causes the dissolution of IMC continuously. As mentioned later in the section of discussion, the migration of Cu atoms within the solder material is much faster than that of Ni atoms. Due to the massive dissolution of Cu atoms within IMC layer, the (Ni,Cu)3Sn4 phase would form at the expense of FeSn2 and (Cu,Ni)2Sn5 during the dissolution process.

Among all the failed SAC/Fe-45Ni solder joints, only one failure mode (Mode I) was detected. Cracks always initiated and propagated along the interface of IMC/solder as depicted in the Fe-45Ni solder joints after 2749 h EM in Fig. 6(g). And the fracture occurred along the FeSn2/SAC interface as enlarged in Fig. 6(h). Also, (Cu,Ni)2Sn5 was seldom observed at Fe-45Ni cathode. However, due to the intrinsic lower Ni concentration and superior barrier effect than Fe-73Ni, (Ni,Cu)3Sn4 was also barely observed at Fe-45Ni cathode. Compared with the thin layer of FeSn2 at cathode, IMCs at the anode were accumulated to tens of microns (Fig. 6(i)). Especially, the thickness of FeSn2 layer and the mixed layer was as thick as 11 μm, which was about seven folds to the FeSn2 layer at the cathode (1.6 μm). Above all, the failure modes varied with the different growth behavior of IMCs for Fe-Ni solder joints, which can all be classified as the crack at the cathodic interface between solder and outer IMC layer.

3.3. Characteristic lifetime determined by Weibull distribution

During the EM test, the resistances of the test vehicles were monitored as a function of time until failure. The resistances fluctuated towards higher or lower imbalances during the incubation time of cracks, and then increased quickly leading to an open circuit in a short time. The higher imbalance was attributed to the formation of voids and simultaneous damage, while the lower imbalance was caused by the recovery process within the solder joints [19,20].

Weibull distribution is one of the most commonly used tools to calculate the lifetime for the reliability test of micro-electronics [21]. And Weibull function is given by the formula [22]:

$$F(t) = 1 - \exp \left[ -\left(\frac{t}{\eta}\right)^{\beta} \right]$$  (1)
where \( F(t) \) is the cumulative failure percentage, \( \eta \) is the scale parameter, \( \beta \) is the shape parameter and \( t \) is failed time for each vehicle. The scale parameter \( \eta \) is also defined as the characteristic lifetime at which 63.2\% of the population has failed. Fig. 7 presents the plots of Weibull distribution for the EM test reliability. The correlation coefficient \( Rho \), the scale parameter \( \eta \) and the shape parameter \( \beta \) for different UBMs are listed in Table 2. The \( Rho \) values among three UBMs are above 0.96, demonstrating a good fitting for the failure data. The value of \( \beta \) has a distinct effect on the failure rate and therefore the failure mechanisms can be identified by its value. When \( \beta > 1 \), the failures become more frequent as the time elapses, and failures of wear-out type are expected. The characteristic lifetimes for Fe-73Ni and Fe-45Ni UBM are 2121 and 2340 h as highlighted by dot lines in Fig. 7. And both lifetimes of Fe-Ni UBMs are over three folds to that of Cu UBM (698 h), indicating an outstanding advantage for Fe-Ni UBMs in EM resistance.

According to the above results, Fe content within the UBM affects the growth of IMC and the lifetime of Fe-Ni solder joints during EM test. Moreover, it was found that the diffusion of atoms was decreased and the lifetime was enhanced with more Fe content within UBM. However, Fe-Ni alloys with the composition above 59 wt% Fe have FCC-BCC phase transition during the preparation process, which affects the property and internal stress of thin film greatly [23,24]. Moreover, Guo et al. [8] had pointed out that the wettability of Fe-48Ni UBM was superior to pure Ni, while the wettability of Fe-25Ni UBM decreased due to the formation of thicker oxide on the surface. So, as a potential UBM material, the Fe element within Fe-Ni UBM should be constricted within an appropriate range. And Fe-45Ni can be regarded as a superior candidate for UBM material.

4. Discussion

According to the observed experimental results described above, fast consumption of Cu cathode and solder voiding led to the failure of SAC/Cu solder joints during EM test. However, there were no solder voids and serrated dissolution within Fe-Ni UBMs after 1000 h current stressing, indicating a better EM resistance of Fe-Ni UBMs. The superior EM reliability of Fe-Ni UBMs lies in two aspects, which are the slower dissolution rate and the restraint of cracks initiation at Fe-Ni cathode. In order to understand the EM mechanism of Fe-Ni UBM, these two aspects were discussed separately. The mass fluxes within Fe-Ni solder joints are illustrated in Fig. 8 schematically. And the solder joint with Fe-Ni cathode in Fig. 8(a) was discussed prominently, while that with Fe-Ni anode in Fig. 8 was served as a comparison.

4.1. Cathode dissolution

There are five types of mass fluxes inside Fe-Ni solder joints: Cu flux \( j_{Cu} \), Ni flux \( j_{Ni} \), Fe flux \( j_{Fe} \), vacancy flux \( j_{V} \) and Sn flux \( j_{Sn} \). With respect to the cathode dissolution, the atomic fluxes of \( j_{Cu} \), \( j_{Fe} \) and \( j_{Sn} \) were discussed, while \( j_{Ni} \) and \( j_{V} \) were ignored since they contributed merely to the cathode dissolution as illustrated in Fig. 8(a). The environmental conditions during EM test contain the heat and current, so atomic fluxes were driven under the interaction of thermal diffusion and EM effect. Therefore, the superscript “CHEM” of \( j \) is used to represent the diffusion term under thermal effect, while the superscript “EM” indicates the drift term due to EM effect.

As for the cathode dissolution, the diffusion term was discussed firstly. The \( j^\text{CHEM} \) can be expressed in the Fick’s first law:

\[
\frac{d}{dx} \left( D \frac{\partial C}{\partial x} \right) = \frac{\partial}{\partial x} \left( j^\text{CHEM} \right)
\]

where \( D \) is the diffusivity and \( \frac{\partial C}{\partial x} \) is the gradient of concentration at the interface. So the \( j^\text{CHEM} \) has a direction pointed to the low concentration area. Therefore, all the \( j^\text{CHEM} \) flux within the solder joints flow from the substrate to solder material. During the aging process, the atomic source of IMCs comes from \( j^\text{CHEM} \). Owing to the addition of Fe-Ni UBMs, the growth of IMCs was suppressed in different levels compared to Cu solder joints as shown in Fig. 2, which demonstrates a smaller \( j^\text{CHEM} \) at SAC/Fc-Ni interface experimentally. And the \( j^\text{CHEM} \) at SAC/Fe-Ni system interface should be lower than that of SAC/Fe-Ni considering the thickness of interfacial IMCs. The diffusivities within SAC/Cu and SAC/Fe-Ni system can be obtained from the parabolic growth of IMCs during the aging test [25]. The determined values for the diffusivity of Cu in Cu_3Sn and Cu_6Sn_5 phase at 150 °C within SAC/Cu system are 3.8 × 10−17 and 3.2 × 10−17 m²/s, respectively. When Fe-Ni UBM was applied, the diffusivity of Cu in (Cu/Fe/3SNi)_5 phase was decreased 76.5% to a value of 7.52 × 10−18 m²/s. The diffusivity of Fe in Sn_2 was 6.24 × 10−19 m²/s and it was two orders of magnitude lower than those IMCs at SAC/Cu interface. Darivach et al. [5] and Zhu et al. [26] had also reported that IMCs at SAC/Fe-Ni solder joints process lower diffusivities and higher activation energies compared to the conventional Cu and Ni UBMs. Beside the \( j^\text{CHEM} \) at the SAC/UBM interface, the \( j^\text{EM} \) makes great contribution to cathode dissolution. While the \( j^\text{EM} \) flux can be described in the formula [27]:

\[
j^\text{EM} = \frac{C}{kT} \frac{D}{e} \rho j
\]

where \( C \) is the concentration, \( D \) is the diffusivity, \( k \) is the Boltzmann constant, \( T \) is temperature and the value is 423 K in this study. \( Z \) is the effective charge, which was composed of the electrostatic charge number and electron wind charge number. The electrostatic charge number represents the direct electrostatic force on the moving ion and hence its value is expected to be the nominal valence of the ion. The electron wind charge number accounts for the electron wind force, which is generally the dominant contribution [28]. The \( e \) is the fundamental charge, \( \rho \) is the resistivity of solvent and \( j \) is the current density which is 1.2 × 10⁴ A/cm² in this study. In order to discuss the influence of EM on cathode dissolution, the fluxes under EM effect are divided into two parts, which are \( j^\text{EM} \) and \( j^\text{EM} \). \( j^\text{EM} \) represents the flux at the SAC/UBM interface, while \( j^\text{EM} \) represents the EM flux within solder material. The effective charge \( Z \) for pure
Fe, Ni and Cu were 2±1, −3.5 and −5.5 ±1.5, respectively [29]. So both $J_{EM}^F$ and $J_{EM}^Ni$ are in the same direction with electron flow, which accelerate the cathode dissolution. It is obviously that $J_{EM}^F$ is in the opposite direction to the electron flow due to the positive effective charge $Z$ of Fe atoms [30]. Therefore, $J_{EM}^F$ partly counteracted with the diffusion term $J_{EM}^{\text{chemical}}$ at the cathode, and slowed down the dissolution process. The growth behavior of FeSn2 supports this conclusion, which was suppressed at the cathode while accelerated at the anode as stated above.

In terms of the dissolution of IMCs, the EM fluxes mainly depended on the product of diffusivity and effective charge number $DZ$ according to Eq. (3), since the concentration can be determined from the atomic ratio within a specific IMC. The values of $Z$ for Cu within Cu$_2$Sn and Cu$_6$Sn$_5$ had been calculated as −26.5 and −26, respectively [28]. But the effective charge $Z$ for Cu, Ni and Fe as solutes within (Cu,Ni)$_5$Sn$_3$ and FeSn$_2$ were seldom reported, which made it difficult to calculate the $EM$ flux at SAC/Fe-Ni interface quantitatively. However, the effect of $Z$ for both (Cu,Ni)$_5$Sn$_3$ and FeSn$_2$ was believed to be not crucial, since the diffusivities of IMCs in Fe-Ni solder joints were one or two orders of magnitude smaller than the IMCs in Cu solder joint as demonstrated above. Moreover, it was further proved by the slow dissolution process for IMCs at Fe-Ni cathode experimentally. Unlike the obvious dissolution of Cu$_6$Sn$_5$ at the cathode, both the dissolution of FeSn$_2$ and (Cu,Ni)$_5$Sn$_3$ were too slow to be detected during the EM test.

In summary, experimental results showed that there is no depletion or serrated dissolution of Fe-Ni cathode even within the failed solder joints after 3000 h EM test. The good resistance on cathode dissolution is attributed to the following two reasons. Firstly, low diffusivity and high activation energy of IMCs at SAC/Fe-Ni interface prevent fast consumption of Fe-Ni cathode. Secondly, Fe atoms transfer in the opposite direction to electron flows, which can suppress the diffusion of Fe-Ni atoms.

4.2. IMC accumulation and crack initiation

Before crack initiation, IMC accumulation happened first due to the migration of atoms, which was closely related to the atomic fluxes within solder material. Since the IMC accumulation was originated from the dissolution of IMC and UBM material at the cathode, the solder joint with Fe-Ni cathodes in Fig. 8(a) was analyzed. For multi-diffusers system, the solute correlation factor $f$ was introduced in the analysis of EM flux, and Eq. (3) was modified as below [29]:

$$J_{EM}^F = C_b \frac{D_{Cu}Z_b e^f}{kT}$$

where the $C_b$, $D_{Cu}$, $Z_b$ represents the concentration, diffusivity and effective charge number of diffusers within solder material. The subscript b represents Cu and Ni atoms in Fig. 8(a), and there is a relationship of correlation factor $f_{Cu} = f_{Ni} = 1$. The other parameters are the same as stated in Eq. (3).

From the above analysis, IMC accumulation was induced by the flux of $J_{EM}^F$ for SAC/Cu solder joint, while the combined flux of $J_{EM}^{Cu} + J_{EM}^{Ni}$ contributes to the IMC accumulation in SAC/Fe-Ni solder joints. From Eqs. (3) and (4), these fluxes can be evaluated by the value of $C_{Cu}D_{Cu}Z_{Cu}$ for SAC/Cu solder joints, and $C_{Cu}D_{Cu}Z_{Cu}Cu + C_{Ni}D_{Ni}Z_{Ni}Ni$ for SAC/Fe-Ni solder joints. The solder material Sn3.8Ag0.7Cu here was simplified into pure Sn in order to evaluate the fluxes.

Within the solder material, Cu, Ni and Fe atoms are regarded as diffusers, while Sn atoms are regarded as the solvent. Due to the strong anisotropy of Sn crystal, the c axis provides a rapid diffusion path for diffusers. However, the polycrystalline diffusivity on average was considered more practical in this study. The diffusivity reported in literature was usually in two directions, which are parallel and perpendicular to the c axis of Sn crystal. And the polycrystalline diffusivity can be determined by the average value of $D$ through the equation: $1/D = 1/D_1 + 2/D_2$, where $D_1$ is the diffusivity along the c axis and $D_2$ is the diffusivity along the perpendicular axis according to the study of Linares et al. [31]. Based on the analysis above, the polycrystalline diffusivities are deduced and the results are given in Table 3 [32–34]. Consequently, the diffusivity for Cu, Ni and Fe within Sn were calculated to be 9.4×10$^{-8}$ cm$^2$/s, 1.9×10$^{-9}$ cm$^2$/s and 2.4×10$^{-10}$ cm$^2$/s at 150°C, which were 10$^{-2}$–10$^2$ times larger than the self-diffusivity of Sn(1.11×10$^{-15}$ cm$^2$/s) as reported [18].

The absolute value of $Z_{Cu}$ within Sn was 2 and $C_{Cu}$ within Sn was 6×10$^{-3}$ wt% as reported [18], While the absolute value of $Z_{Ni}$ was 0.5 [35], and $C_{Ni}$ was as low as 5×10$^{-8}$ wt% at room temperature [33]. It is easy to deduce the relationship of $C_{Cu}D_{Cu}Z_{Cu}Cu > C_{Cu}D_{Cu}Z_{Cu}Cu + C_{Ni}D_{Ni}Z_{Ni}Ni$ from the above data. Therefore, the $J_{EM}^F$ flux in SAC/Fe-Ni solder joints was theoretically smaller than that in SAC/Cu solder joints, which implies less atom migration within the solder.

Notably, $J_{EM}^F$ was not considered within the analysis (also see Fig. 8), due to the following two reasons. On the one hand, the
atomic source of EM flux within solder material comes from the dissolution of IMC and substrate. Since Fe atoms transfer in the opposite direction to electron flows, there is no supply of Fe atoms from the PCB side with Cu pad and Cu$_6$Sn$_5$ upon. On the other hand, the diffusivity of Fe atoms within the solder material was two orders lower than that of Cu atoms, which can be ignored. Actually, only the migration of Cu atoms within the solder material was obvious, both the Fe and Ni flux were too small to be observed in the experiment.

As atoms migrate towards the anode within solder material, the vacancy flux $J_v$ was functioned. Compressive stress was built up when the atoms transferred towards the anode along electron flow. A lower vacancy concentration formed at the anode and a higher vacancy concentration formed at the cathode side according to the Nabarro–Herring model [36], which induced compressive stress at the anode. Thus the $J_v$ was set up and flowed from the anode to cathode. Vacancy flux can annihilate at dislocations, and can also condense into voids. As Seitz [37] proposed based on thermodynamic calculations, an excess vacancy of twice the equilibrium concentration was responsible for the steady formation of voids. Therefore, $J_v$ is believed to be the main reason of solder voiding and crack initiation during long-term stressing. The relationship between $J_v$ and the migration of atoms can be expressed with equation [29]:

$$J_v = J_{b}^{EM} + J_{Sn}^{EM}$$

(5)

The value of $J_v$ is equal to the EM flux of both solute and solvent within the solder material, but in the opposite direction. As for the solvent Sn, the $J_{Sn}^{EM}$ is a constant value according to Eq. (3), since the solder material is the same within Cu and Fe-Ni solder joints. Therefore, the $J_v$ within Fe-Ni solder joints is smaller due to the smaller value of $J_{Sn}^{EM}$ from Eq. (5). As a result, it took long time for the process of vacancy accumulation and void formation at Fe-Ni cathode, which was also responsible for the extended lifetime of Fe-Ni solder joints.

Above all, the diffusion term $f^\text{CHEM}$, the EM term $f^\text{EM}$ at the SAC/UBM interface and the EM term $f^\text{EM}$ within solder material were analyzed, respectively. With respect to the cathode dissolution, the $f_{\text{CHEM}}^{\text{CHEM}}$ and $f_{\text{EM}}^{\text{EM}}$ of different solder joints were discussed, and smaller values were obtained for Fe-Ni UBM solder joints compared with Cu. It was concluded that Fe element plays a key role in the resistance of cathode dissolution. With respect to the IMC accumulation, the $f_{\text{IMC}}^{\text{EM}}$ was considered. The $f_{\text{EM}}^{\text{EM}}$ and $J_v$ flux in SAC/Fe-Ni solder joints were smaller than that of SAC/Cu solder joints, which led to the less IMC accumulation and crack initiation.

5. Conclusions

The EM behaviors of Fe-Ni solder joints were investigated, and remarkable differences from those in SAC/Cu solder joints were revealed. Rapid dissolution of Cu cathode and solder voiding resulted in quick interfacial failures in SAC/Cu solder joints, while Fe-Ni cathodes showed no failure signs after 1000 h EM. According to the in-situ monitoring of resistance on three different UBM solder joints, the characteristic lifetimes of both Fe-Ni UBMs (2121 h for Fe-73Ni and 2340 h for Fe-45Ni UBM) are all over three times than that of Cu UBM (698 h), which indicates an outstanding EM resistance for Fe-Ni UBM. As EM test lasted over 1000 h, failures within Fe-73Ni solder joints differ with the growth of IMCs, which can be categorized as two modes: firstly cathode crack initiated at the interface of IMC/solder, and secondly the cathode cracks at the interface of V-shape IMC/solder. Meanwhile, only the first failure mode was detected in Fe-45Ni solder joint.

The mechanism for superior EM reliability of Fe-Ni solder joints was discussed considering two factors. Firstly, cathode dissolution was suppressed by the slower thermal diffusion and smaller EM flux at SAC/Fe-Ni interface. Secondly, due to the restraint of vacancy flux within Fe-Ni solder joints, the cracks at the cathode were also suppressed, which greatly extended the lifetime. According to experimental results and comprehensive discussion in this study, Fe-45Ni alloy can be regarded as a candidate for novel UBM material with superior resistance to electromigration.

Acknowledgements

This work was financially supported by the National Key Research and Development Program of China (Grant No. 2017YFB0305001), the National Natural Science Foundation of China (Grant Nos. 51401218 and 51171191), and the Osaka University Visiting Scholar Program (Grant No. J113504902). We are appreciating the help from the JCAP (Jiangyan Changdian Advanced Packaging Co., Ltd) in providing the technology of Wafer level chip scale package (WL CSP) during sample preparation.

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