Effect of Sn grain orientation on formation of Cu₆Sn₅ intermetallic compounds during electromigration

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Abstract

The effects of Sn orientation and grain boundary misorientation on formation of Cu-Sn intermetallic compounds (IMCs) during electromigration were investigated. Significant anisotropic diffusion of Cu in Sn grains was observed. Interfacial Cu-Sn IMCs may grow rapidly, dissolve, or remain intact, depending on the angle of c-axis of Sn grains with the electron flow. In addition, grain boundaries did not play an important role in Cu diffusion because they are mostly cyclic twins.

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- Intermetallic compounds
- Electromigration

1. Introduction

Beta-Sn (β-Sn) has a body-centered tetragonal structure and possesses anisotropic, thermal, mechanical and diffusion properties [1–4]. Sn grains are the matrix of main-stream Pb-free solders and thus the Sn grain orientation affect seriously the reliabilities of flip-chip joints and microbumps [5–7]. In particular, the effect of Sn grain orientation on electromigration (EM)-induced failure is a very important issue in flip-chip solder joints [6–9]. It is reported that Sn grains with c-axis cause fast formation of Ni₃Sn₄ intermetallic compounds (IMCs) and early failure in the solder joints [6]. However, anisotropic diffusion of Cu atom in Sn grains is seldom examined. In addition, Tasooji et al. reported that the effect of Sn grain boundary misorientation on electromigration is more significant than that of Sn grain orientation owing to the markedly higher diffusivity along grain boundary than that of lattice [10]. They found that Cu atoms diffused along high-angle grain boundaries and facilitated the dissolution of under bump metallization (UBM). Whether grain boundaries diffusion plays an important role in electromigration of solders is not clear. In this study, Cu/Sn-2.3Ag/Cu microbumps are fabricated and electromigration tests were conducted under current density of 4 × 10⁴ A/cm² and 165 °C. Electron backscattered diffraction (EBSD) was utilized to investigated the effect of grain orientation and grain boundary on formation Cu₆Sn₅ IMCs.

2. Experimental

Cu/Sn-2.3Ag/Cu microbumps comprising 7 µm-Cu/16 µm-SnAg/ 7 µm-Cu and of 30-µm diameter were fabricated using thermal-compression bonding (TCB). The bonding of 10 N was achieved at 250 °C for 3 s. The sample was then cooled by an air gun at a cooling rate of about 10 °C/s.

A Daisy chain layout consisting of 40 microbumps was adopted for electromigration tests. The applied current density was 4 × 10⁴ A/cm² at 165 °C. Current stressing was terminated when the resistance of the layout reached 2% of its initial value. After grinding and polishing, the microbumps were analyzed utilizing backscattered electron image (BEI, Supra 55 FE-SEM, Zeiss), and the Sn grain orientation was examined using EBSD (Oxford, equipped in Supra 55 FE-SEM, Zeiss) orientation image mapping (OIM) in the normal direction (ND, the direction vertical to the Si substrate). Image processing was conducted with TSL OIM Analysis 7. For easy understanding of the relationships between c-axis and electron flow in the microbumps, α-angle defined as the angle between the c-axis of Sn and ND is adopted to describe the orientation of Sn grains in this study.

3. Results and discussion

When the α-angle exceeds 70°, no obvious IMC formation was observed after electromigration tests. Fig. 1(a) shows the as-fabricated Cu/Sn₂-3Ag/Cu microbump. The thicknesses of Cu₆Sn₅ IMCs at the top and the bottom of Cu-solder interface are 1.5 and 2.97 µm, respectively. The reason for the thicker IMC on the bottom side is attributed to Cu thermomigration during TCB. Fig. 1(b) and (c) presents the
microstructures of two microbumps after the electromigration test with opposite electron flow of $4 \times 10^4$ A/cm$^2$ at 165 °C for 65 h. Comparing Fig. 1(b) and (c) with Fig. 1(a) revealed no obvious changes in interfacial IMC thickness, regardless of the directions of electron flow. Fig. 1(d) illustrates the EBSD OIM image for the microbump in Fig. 1(b). The image pole figure (IPF) is also shown in the figure. The Sn lattice is labeled schematically in the grain. The solder consists of a single grain with $\alpha$-angle of 81°. Fig. 1(e) presents the OIM image of the microbump in Fig. 1(c). There are four grains in this cross-sectional structure, but all of them have $\alpha$-angles exceeding 72°. In addition, the grain boundaries in this microbump are all cyclic twins, as labeled in Fig. 1(d), and there is little IMC formation along the cyclic-twin boundaries. Owing to the high-angle grains and cyclic twins, the diffusion of Cu in the two microbumps is very slow, resulting in no obvious change in interfacial IMC thickness of the microbump after current stressing. However, extensive formation of Cu-Sn IMCs occurred in the Sn grains with low $\alpha$-angles.

Fig. 2(a) and (b) presents two microbumps after the same current stressing conditions with an opposite electron flow. Extensive formation of Cu$_6$Sn$_5$ IMCs was observed with serious dissolution of Cu in the cathode end of both microbumps. Some of the IMCs even bridged the joints. Fig. 2(c) shows the EBSD results for the microbumps in Fig. 2(a). The remaining grains with extensive IMC formation have $\alpha$-angles of 13° and 10°. However, the grains on the left-hand side have $\alpha$-angles of 82° and 59°, and they did not have obvious IMC growth. Fig. 2(d) illustrates the grain orientation for the remaining grains in Fig. 2(b). As can be seen, the grains have low $\alpha$-angles of 17° and 25°. Taken together, these results indicate very rapid IMC formation in grains with low $\alpha$-angles and different IMC formation behavior in grains with intermediate $\alpha$-angles.

![Fig. 1](image1.png)

![Fig. 2](image2.png)
Fig. 3(a) and (b) presents SEM images for two microbumps containing grains of intermediate \( \alpha \)-angles after the same current stressing conditions. It is interesting to note that the Cu-Sn IMC on the cathode end dissolved while that on the anode end grew slightly. The measured Cu-Sn IMC thickness is 0.5 \( \mu \)m and 3.21 \( \mu \)m on the cathode and anode end, respectively. The Cu-Sn IMC on the cathode is thinner than that of the as-fabricated sample shown in Fig. 1(a). The OIM images in Fig. 3(c) and (d) reveal that the grains in these two microbumps have \( \alpha \)-angles ranging from 46° to 61°. In addition, the grain boundaries in these two microbumps are cyclic-twin boundaries, as labeled in red lines in the figure.

To further examine the percentage of cyclic-twin boundaries, the grain boundary structure in 15 as-fabricated microbumps was analyzed. Fig. 4(a)–(d) depicts the OIM images of four microbumps, respectively. As can be seen, most of the grain boundaries consist of twin structures, as labeled in red lines in the figure. Fig. 4(e) summaries the results, indicating that the misorientation of grain boundary locates mostly at 55–65°. It has been reported that the misorientation of cyclic-twin boundary is 57.2° and 62.8° for \{101\} and \{301\} planes, respectively [11]. The percentage of cyclic-twin boundaries in one microbump can be as high as 85%. Twin boundary is a coherent boundary; hence, Cu diffusion in the cyclic-twin boundary is not fast. This study did not observe rapid Cu diffusion or Cu-Sn IMC formation in Sn-Ag microbumps with only a small percentage of cyclic-twin boundaries in Sn-Cu solder joints [11]. Thus, grain boundary diffusion in Sn-Cu solder joints has significant influence on diffusion of Cu during electromigration [10].

It is reported that Cu atoms have extreme anisotropic diffusion in Sn grains [12]. We perform the following quantitative analysis to correlate the relationship of anisotropic Cu diffusion and the structure of Sn grains during current stressing. The Cu diffusivities along c-axis (\( D_{c,Cu} \)) and a-axis (\( D_{a,Cu} \)) of Sn are given below: [12]

\[
D_{c,Cu} = 1 \times 10^{-3} \exp \left[ -\frac{4000}{RT} \right] \\
D_{a,Cu} = 2.4 \times 10^{-3} \exp \left[ -\frac{7900}{RT} \right]
\]

Where \( R \) is Boltzman’s constant and \( T \) is temperature. At the EM testing temperature of 165 °C, the calculated Cu diffusivity is \( 1.0 \times 10^{-5} \) cm²/s and \( 2.7 \times 10^{-7} \) cm²/s for Cu atoms along the c-axis and a-axis, respectively. That is, the Cu diffusivity along the c-axis of Sn grains is 37 times faster than that along the a-axis of Sn grains. In addition, when the Cu flux diffuses at an \( \alpha \)-angle to the c-axis of Sn grains, \( D_{\alpha} \), the Cu diffusivity can be expressed as: [4]

\[
D_{\alpha} = D_{c}\cos^{2} \alpha + D_{a}\sin^{2} \alpha
\]

In the present study, the Sn grains have \( \alpha \)-angles ranging from 10° to 82°. We calculate the Cu diffusivities of 13°, 55°, and 81° Sn grains, and the diffusivity is \( 9.5 \times 10^{-6} \) cm²/s, \( 3.5 \times 10^{-6} \) cm²/s, and \( 5.0 \times 10^{-7} \) cm²/s, respectively. The diffusivity of Cu atoms in the 13° Sn grain is 19 times faster than that in the 81° Sn grain. This diffusivity difference causes the variation in the growth rate of interfacial Cu-Sn IMCs.

The effect of Sn grain orientations on interfacial formation can be summarized as follows. For Sn grains with small \( \alpha \)-angles, the interfacial Cu-Sn IMCs and Cu UBM on the cathode end dissolve rapidly because of high diffusivity of Cu in the Sn grains, and huge amount of Cu-Sn IMCs form on the anode end. For Sn grains with intermediate \( \alpha \)-angles, the thickness of the Cu-Sn IMCs on the cathode end decreases significantly, but the Cu UBM does not dissolve much due to intermediate diffusivity of Cu in the Sn grains. The Cu-Sn IMCs on the anode end grow slightly thicker. Yet, the thickness of the interfacial Cu-Sn IMCs on both cathode and anode ends almost remains unchanged after the current stressing for high \( \alpha \)-angle Sn grains, because the diffusivity of Cu in Sn is very low. This anisotropic growth of Cu-Sn IMCs occurs in systems of Sn-based solders and Cu metallization under current stressing. Because the Sn-based solders are the main stream materials and Cu serves as a popular metallization material in microelectronic packaging industry, the anisotropic growth of Cu-Sn IMC is a generic issue in interconnects of microelectronic devices.

4. Conclusion

This study concludes that Sn grain orientation plays a critical role in the growth of Cu-Sn intermetallic compounds during current stressing.
For Sn grains with \( \alpha \)-angles lower than 25°, Cu-Sn IMCs grew very fast during electromigration. On the other hand, for Sn grains with intermediate \( \alpha \)-angles, Cu-Sn IMCs on the cathode end dissolved, and migrated to the anode side, resulting in slightly growth of Cu-Sn IMCs on the cathode end. However, the thickness of interfacial IMCs did not change in Sn grains with a high \( \alpha \)-angles. This is because Cu diffusion was very slow in high-\( \alpha \)-angle Sn grains. In addition, for Sn-Ag solder joints, most of the grain boundaries consist of cyclic twins, and they are not fast diffusion paths for Cu atoms. Therefore, grain-boundary diffusion of Cu is less important than Sn orientation in the formation of Cu-Sn IMCs during electromigration.

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