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Effects of anisotropic β-Sn alloys on Cu diffusion under a temperature gradient

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Abstract

The diffusion mechanism of Cu in a thin layer of Sn–3.5Ag sandwiched between two Cu foils was systematically investigated under a temperature gradient of 2200 °C cm^{-1}. Experimental observation and theoretical derivation reveal that the microstructural evolutions induced by thermomigration are significantly affected by the tetragonal anisotropy of Sn. The thermomigration flux of Cu increased with the squared value of cos α, the angle between the *c*-axis of the Sn grain and the temperature gradient. When the *c*-axis of the Sn grain was parallel to the temperature gradient, a larger thermomigration flux of Cu was induced and the Cu atoms migrated from the hot end toward the cold end. This tended to form a prominent asymmetrical microstructure and cause failure: serious dissolution of intermetallic compounds (IMCs) and excessive consumption of Cu foil occurred at the hot end whereas abnormal accumulation of IMCs was observed at the cold end. Instead, when they are perpendicular, thermomigration would be mitigated due to the lower induced flux. No failure or symmetrical growth of IMCs was found at either interface.

Keywords: Thermomigration; Lead-free solder; Under bump metallization; Sn grain orientation; Intermetallic compound

1. Introduction

Thermomigration (TM), one kind of mass transport induced by a temperature gradient, has been regarded as one of the critical reliability issues for electronic packaging technology. In flip-chip technology, thermomigration of solder joints has been observed to occur because of electromigration [1–4]. When the solder joints are current-stressed, the resultant Joule heating from the chip side is higher than that from the substrate side due to the geometrical configurations of the electronic package [4,5], causing a non-uniform temperature distribution in solder joints. In addition, the effect of current crowding leads to the chip side of solder joints being hotter than the substrate side. Consequently, a temperature gradient is established across solder joints. Many investigations have reported that a temperature gradient of 1000 °C cm^{-1} is sufficient to trigger thermomigration and thermomigration can cause element redistribution in solder alloys [2–4,6,7]: Sn atoms move to the hot end while Pb and Bi atoms move toward the cold end. The under-bump-metallization (UBM) element, such as Cu and Ni, tends to migrate under a temperature gradient as well. Chen et al. [8,9] observed the temperature-gradient-induced dissolution of the Cu UBM layer at the hot end and the direction of Cu migration toward the cold end. They also found that the critical temperature gradient to trigger thermomigration of Cu atoms in Pb-free solders was ~400 °C cm^{-1} [8]. Moreover, in Ouyang's study [10,11], Ni atoms were observed to be driven from the hot end toward the cold end in micro-solder joints when a temperature gradient existed.

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Recently, a three-dimensional integrated circuit (3-D IC), a vertically integrated system, has been regarded as one good solution to fulfill the demand for both the trend of miniaturization for electronic devices and for the better performance in the electronic packing technology. Accompanied with the development and implementation of the 3-D IC, packaging technology is now facing new problems and challenges. One problem is the amount of Joule heating generated in 3-D IC packaging; lots of heat will be produced when many transistors work simultaneously inside a compact vertically stacked module. If the heat is dissipated from the surfaces of the module, a temperature difference between the surface and the inner parts of the module could create a temperature gradient across the module. In addition, the peak temperature of a working 3-D IC module has been reported to be much higher than that of flip-chip technology [12], leading to faster atomic diffusion. Moreover, the height of solder joints will drop drastically from a few hundreds of micrometers to only a few micrometers in 3-D IC packaging technology. The reduction in height and the higher peak temperature may facilitate the occurrence of thermomigration in 3-D IC. Hence, thermomigration is believed to be a potentially serious reliability problem in the development of 3-D IC packaging technology.

Another emerging concern in the development of the 3-D IC packaging technology is the anisotropic nature of Sn with a body-centered tetragonal (bct) crystal structure [13]. Sn is a major component of Pb-free solders. When a solder joint is significantly downsized into a few micrometers, it may be composed of only a few Sn grains. It now becomes important to understand how anisotropic Sn affects the performance and the reliability of solder joints once only one or two grains exist in the joint. The influences of the anisotropy of Sn on failure mechanism of Pb-free solders during electromigration have been extensively investigated [14–21]. When electrons flow along the *c*-axis of the Sn grain in the solder joints [17,20], fast dissolution of the UBM layer occurs. Pancake-type voids of solders have been observed when electrons flow perpendicular to the *c*-axis of the Sn grain. The growth of IMCs during current stressing was also found to be related to the direction of the *c*-axis of the Sn grain [18,19,21]. However, no study has yet reported on how the anisotropic β-Sn affects the diffusion behavior and interfacial reaction in the Pb-free solders under a temperature gradient.

In the present work, we systematically studied the relation between the anisotropy of Sn and the thermomigration behavior of Cu in Pb-free solders when Sn–3.5Ag solders reacted with Cu UBM layers. Through microstructural examination using scanning electron microscopy (SEM) and the aid of electron backscatter diffraction (EBSD) analysis, the effect of anisotropic Sn on Cu atomic diffusion as well as on the Cu–Sn interfacial reaction in Pb-free solders under a temperature gradient was elucidated. The corresponding theoretical model was also developed to quantitatively explain the fundamentals of thermomigration of Cu regarding grain orientation. The findings provide not only further insight into the kinetic analysis of diffusion anisotropy under a temperature gradient, but also guidance to the preferred grain orientation for Pb-free soldering technology in next-generation electronic products.

2. Experimental

The samples were fabricated as a sandwich structure: Cu/Sn–3.5Ag solder/Cu. To achieve better wettability, Cu plates (5 × 5 × 1 mm) were first ground, polished and cleaned in advance to remove surface oxides. The Sn–3.5Ag solder pastes were then uniformly applied onto the flat Cu surfaces. The use of solder paste also helps to obtain better wettability and stronger connection due to the incorporation of a certain amount of flux in the paste, making it less easy to form voids at the interface between the solder layer and the substrate during the soldering process. Next, two Cu plates with a thin layer of solder paste on each side were assembled and reflowed on a hot plate. The peak temperature of the reflow process was 260 °C and the duration was 60 s. The thickness of the solder layer varies from 282 to 285 μm. After assembly, to facilitate an observation of the effect of grain orientation on the thermomigration test, samples were post-annealed at 150 °C for 48 h to coarsen Sn grains.

Table 1 lists the test conditions. As depicted in Fig. 1, a thermomigration test was conducted by placing samples in between a heat source and a heat sink device, following the method developed by Ouyang et al. [10,11]. Thermocouples were respectively attached to both devices to continuously monitor temperature variations during the tests, and a feedback system was utilized to maintain the temperature of each device. The heat source was fixed at 200 °C and the heat sink maintained at 100 °C. The temperature gradient of the samples was established from the upper Cu plate toward the bottom Cu plate. To understand the temperature gradient across the solder layer, the finite element method was employed. The thermal boundary conditions were set based on the recorded temperature of the thermocouple of each device. The top surface of the upper Cu plate was set to be 473 K (200 °C) and the surface of bottom Cu plate attached to the heat sink was set to be 373 K (100 °C). The thermal conductivity of Cu and Sn–3.5Ag used in the simulation is 389 W m^{-1} K^{-1} and 33 W m^{-1} K^{-1}, respectively [22,23]. For the sake of comparison, some samples were subject to isothermal treatment at 150 °C for different durations.

After tests, scanning electron microscopy (FE-SEM, JSM-6500F, JEOL) and energy dispersive X-ray

Table 1
Test conditions.

	Initial aging	Test condition
Thermomigration test (TM-test)	150 °C for 48 h	Heat source: 200 °C Heat sink: 100 °C
Isothermal aging test	150 °C for 48 h	150 °C