

Study of Formation and Change of Intermetallic Compounds in Cu-Au and Au-Al Systems for Copper on Gold Bonding

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Abstract

Copper (Cu) ball on gold (Au) bump (COG) bonding is developed as a practicable approach to solving the challenges posed by Cu wire bonding on large-scale integrated circuit devices. In the COG bonding, there are two interfaces, Cu-Au and Au-Al couples, which is totally different from either Cu or Au wire bonding. In this paper, the COG bonding is studied on an experimental chip of 69μm bond pad opening and 4-layer central via pattern design with current wire bonders.

Tests of wire pull, ball shear and crater are adopted in investigating the bonding strength at the interfaces and the potential damage of the underlying metals of bond pads after the COG bonding. The intermetallic compounds (IMC) formation at the two interfaces, Cu-Au and Au-Al couples, are studied on the cross-sectioned assembled samples. Two kinds of stress tests, High Temperature Baking (HTB) and Temperature Cycle (TC) are used to investigate the IMC change and growth.

The results show that qualified bonding strength on all of bond pads exists and no damage such as crater is observed on the underlying metals of the bond pads after chemical etching. At the Au-Al interface, a comparable Au-Al IMC is formed on as-bonded samples, and it gradually grows thick after the stress tests and its corresponding content also changes along with temperature and time. But in contrast there is no observable formation of Cu-Al IMC at the Cu-Au interface on as-bonded samples. Undergoing 1008 hours HTB at 175°C, only a very thin Cu-Au IMC appears at the Cu-Au interface. After all, the Cu-Au IMC appearance hardly affects the IC's mechanical performance.

Key words — COG, IMC, Inter-diffusion, Crater and Void

1. Introduction

In microelectronic packaging, thermosonic bonding technology plays a leading role in making electrical interconnections between IC chips and lead frames or substrates. Gold (Au) wire is the most popular material used in thermosonic bonding. With gold price continuously soaring and IC packaging cost competition, copper (Cu) wire is generally regarded as an alternative interconnection material to replace gold wire. Cu wire has a lower price and better mechanical/electrical characteristics than Au wire. However, its well-known high hardness poses big challenges when introducing Cu wire bonding on large-scale ICs because this high hardness tends to induce assembly defects such as crater, peeling and underlying crack of bond pads. Thereby, Cu wire has been limited to discrete parts and low-scale ICs for high-volume production till now.

A new wire bonding approach called COG (Copper ball on Gold bump) bonding is developed to solve the

challenges in direct Cu wire bonding so that it may emerge as a practicable technology for large-scale ICs. In the COG bonding, at first, an Au bump is bonded on bond pad, and then a Cu ball is micro-welded on the top of the Au bump. Both steps are implemented with existing wire bonders. As gold is much softer than copper, the Au bump serves as a cushion to absorb majority of mechanical stress from the Cu wire bonding by its body deformation. With major stress absorption, the bond pad in chip only experiences partial stress and the challenges of the direct Cu wire bonding may be solved. Fig.1 shows the wire bonding process flow of the COG bonding.

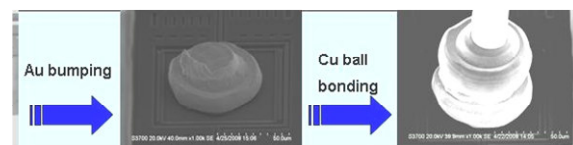


Fig.1 Wire bonding process flow of the COG bonding

In conventional Au wire bonding, only single interface of intermetallic compound (IMC) exists between Au ball and Al metallization layer on chip. Characterization of Au-Al IMC formation and growth through reliability test was studied and reported in many published literatures [1][2][3]. A visual Au-Al layer ranging from 0.3 μm to 1 μm can be observed on as-bonded devices after thermosonic bonding done, and then an obvious Au-Al IMC growth through entire assembly and reliability tests, especially with high temperature baking is presented. In the COG bonding, there exist two IMC interfaces, Au-Al and Cu-Au couples at the first bonds, which are significant different from conventional Au wire bonding. Thereby, there is a general concern with formation of the IMC of the Cu-Au couple after thermosonic bonding and its growth through entire assembly and reliability tests.

In the present study, formation and change of IMCs at both Cu-Au and Au-Al couples have been investigated experimentally. The experiment method is first described. Follow it are the detailed integrity assessment of as-bonded samples assembled by the COG bonding, formation of Cu-Au and Au-Al IMCs in as-bonded samples and growth of the IMCs. The conclusions are drawn in the end.

2. Experimental Description

All experimental samples were built by an upgraded Kulicke & Soffa wire bonder with a supplementary gas flow tool. The electrode is placed in a horizontal glass tube with a hole. The tube was filled by shielding forming gas of 95vol% N_2 gas and 5vol% H_2 gas, and capillary can go through the tube when bonding Cu wire. A 1mil diameter Cu wire with purity of 99.99wt % was adopted in the experiments. The Cu wire has a break load range of 11-13gf and a hardness of 60-70Hv. The experimental chip used for the COG bonding has a BOA (Bonding on Active circuit) design with 4-layer-structure bond pads and 69 μm bond pad opening size. For this BOA design, the bond pads have a central via pattern for internal underlying metal structure and a thickness of $\sim 8\text{K}\text{\AA}$ for top metallization layer of 99.5% Al and 0.5% Cu. By Experiment of Design (DOE) approach, bonding parameters for Au bump were finalized to achieve Au bumps of average 57 μm diameter with a compression rate of 25% (ball height vs. ball diameter) prior to Cu wire bonding, and bonding parameters for Cu wire bonding on Au bump were finalized to achieve Cu

bonded balls of an average 56 μm diameter with a compression rate of 55%.

Temperature can significantly affect behavior of IMC growth on as-bonded balls. High temperature can promote atomic diffusion at the two interfaces of Au-Al and Cu-Au couples. According to JEDEC criteria, two reliability tests, High Temperature Baking (HTB) and Temperature Cycle (TC) were chosen to investigate the IMC change for the large-scale IC's reliability assessment with the COG bonding. The HTB was performed on the molded experimental samples in a convection oven at 175°C for up to 1008hours. The TC was conducted between -65°C and 150°C for up to 1000cycles on the molded experimental samples. In order to clearly observe IMC formation and change, cross-sectioned samples were prepared with a JEOL's SM-09010 cross section polisher. This polisher can minimize sample damage, smearing and deformation.

In crater inspections, aqueous solution of 85% phosphoric acid was used to disclose the barrier metal layer underneath Al metallization of bond pads to check any crater destruction.

3. Results and Discussions

Integrity Assessment on As-bonded Samples: Fig.2a shows a SEM panoramic image taken on a typical sample using the COG bonding approach. An amplified image of a typical COG bonded ball on bond pad is shown in Fig.2b. By visually inspecting 48 as-bonded samples, it was found that Cu bonded balls on Au bump had an average 56 μm diameter and a compression rate of about 0.55 under the optimized bonding parameters. The Au bump's ball diameter were enlarged to average 63 μm from previous average 57 μm ball diameter after undergoing second time compression as copper balls were bonded on their top surface. After all, the whole body of each Au bump and Cu ball is fully within bond pads with qualified clearance.

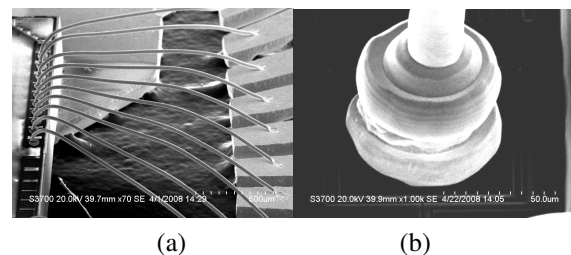


Fig.2 Typical SEM images of the COG bonding (a) panorama (b) a bonded ball.

Three tests, wire pull, ball shear and crater, were conducted to the experimental samples to investigate overall integrity of the as-bonded COG balls. Wire pull test with the hook located at the top of the wire loop was conducted on 48 bonded wires to evaluate the bonding strength at Cu-Au interface. The collected data show an average value of 12.43 gram with a standard deviation of 1.12grams shown in Fig.3, which is 9.43grams higher than the requirement for 1mil wire in JEDEC. Furthermore, failure modes are wire broken at wire neck only. With the satisfied pull force of average 12.43grams and the acceptable failure mode, it may conclude that the joint force at the Cu-Au interface completely meets the criteria for IC's mechanical performance.

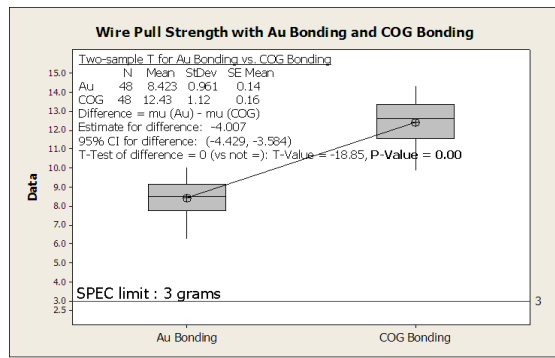


Fig.3. Chart of comparison of wire pull strength between COG bonding and Au bonding

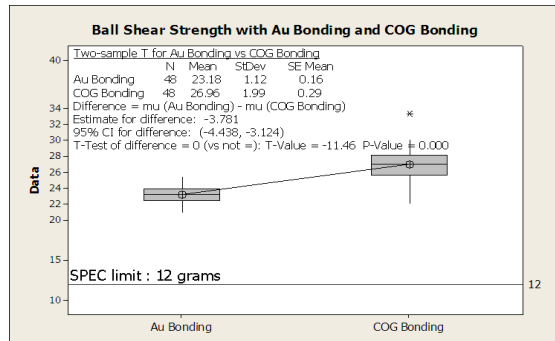


Fig.4. Chart of comparison of ball shear strength between COG bonding and Au bonding

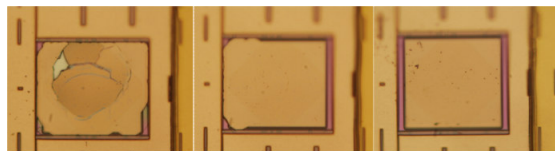


Fig.5 Typical OM images of crater test with Cu wire bonding (left), COG bonding (middle) and Au wire bonding (right)

Ball shear tests and crater tests were also adopted to evaluate the bonding performance of the Au-Al

interface and integrity of underlying metals underneath Al metallization of bond pads. The ball shear force was collected on 48 Au bumps and it is 3.8grams higher than that of the normal Au bumps measured before bonding Cu ball on them shown in Fig.4. This increase of the shear force is attributed to the Au bumps' diameter increase by 10%, which was caused by the second time press when conducting Cu ball bonding on Au bumps. The increase of the contact surface due to the diameter increase raises the shear force. As a result, the increase of ball shear force may reveal that the bonding strength of the Au-Al interface adopting the COG bonding mainly depends on Au bumps' first-time micro-welding on Al metallization, and both mechanical stress and ultrasonic vibration from Cu ball bonding hardly affects the performance of the Au-Al joint interface significantly. So, the integrity of the Au-Al interface is mostly determined by the bonding parameters for Au bumps. In crater tests, the result showed there was no any crater observed among 5 chips taken randomly, and the appearance of the barrier layer of bond pads with the COG bonding was the same as that of Au wire bonding. On the contrary, a popular occurrence of crater was observed among direct Cu wire bonding on the same chips. Fig.5 shows typical images of the disclosed underlying metal in Cu wire bonding, COG bonding and Au wire bonding respectively.

The reason for crater occurrence in Cu wire bonding are as follows: first, Cu has a higher surface hardness than Au due to its thermal-physical characteristics; second, Cu also exhibits larger strain hardening effect at higher strain rate; and finally, the experimental chips have a only 8kÅ-thick Al metallization, which is a standard thickness design for large-scale ICs. When Cu ball is bonded on Al metallization, most Al metal in the bonding region is pushed out of the region. The Cu bonded ball may directly touch the underlying metals with bond force and thermosonic vibration. Consequently, craters tend to occur underneath Al metallization. On the contrary, in the COG bonding, a gold bump formed on Al metallization prior to Cu ball bonding is softer than Cu ball. When performing Cu ball bonding, the formed Au bump as a supporting part is doomed to have an obvious deformation when welding Cu and Au balls together. The Au bump's body deformation inevitably absorb majority of mechanical stress from Cu ball bonding so that only rest of mechanical stress are transmitted to the Au-Al interface through the Au bump. Therefore, risk of crater occurrence is significantly mitigated. When the transmitted stress is less than the withstanding capability of the

underlying metals of the bond pads, the craters are avoided.

Formation of Cu-Au and Au-Al IMCs in As-bonded

Samples: Fig.6 shows the cross-sectioned image of a molded sample with both Cu-Au and Au-Al interfaces using the COG bonding. At the interface between the Au bump and the Al metallization, a thin “Gray” Au-Al IMC layer can be clearly observed under 1000X OM. However, there is no clear evidence of Cu-Au IMC layer at the interface between the Cu bonded ball and the Au bump.

When adopting thermosonic bonding, three modes of energies, bond force, heat and ultrasonic vibration are employed to scrub both Au Free Air Balls (FAB) on Al pads and Cu FABs on Au bumps. At the microscopic level, two bonding surfaces are deformed and interlocked during scrubbing. This induces an initial bonding at the two joint metallic surfaces. In addition, heat from both external supply and friction produced by scrubbing may result in atomic dissolution and diffusion, which usually form intermetallic products at the interfaces. Nucleation of the intermetallics is generally regarded as an indicator for IMC formation [4]. The nucleation of IMCs fully relies on deformation of solid, supplied energies and atomic inter-diffusion of the bonding elements. Therein, the atomic inter-diffusion plays a key role in the formation of the intermetallics. And atomic properties of the bonded elements have significant effects on their atomic inter-diffusion.

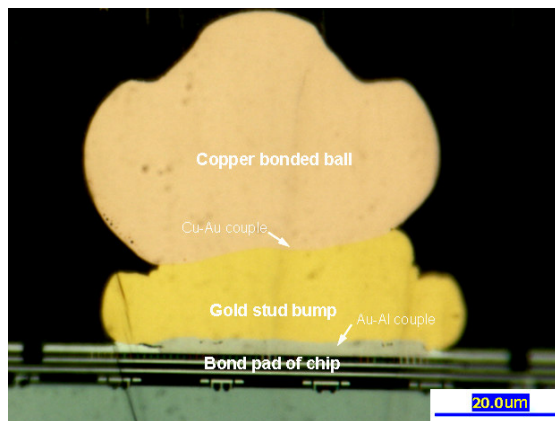


Fig.6 OM images of a typical cross-sectioned samples that has undergone encapsulation and 5 hrs PMC.

For the three elements, Al, Cu and Au, they are all “fcc” crystal structure. Their atomic radii are 0.143, 0.128, and 0.144nm respectively, and so the Cu atom

is 11.1% smaller than that of Au and the Au atom is 0.7% larger than that of Al. According to Hume-Rothery rule, extensive substitutional solid solution occurs only if the relative difference of the atomic diameters (radii) between the two species is less than 15% and a large difference in electronegativity is more likely to form an intermetallic compound instead of a substitutional solid solution. In the Au-Al couple, they have very similar atomic radii so that atomic inter-diffusion by substitutional solid solution easily proceeds without strain of crystal lattice. Moreover, Au has much higher electronegativity than Al (2.54 vs. 1.61). As a result, these lead to form intermetallic products that are stable at the interface of the Au-Al couple. However, in the actual wire bonding process, two different metals are bonded together in a very short time in their solid state. An overall equilibrium is hardly reached within such short process and supply limitation. From the equilibrium phase diagram shown in Fig.7, it may be deduced that multiple intermetallic products comprising Au_4Al , Au_8Al_3 and Au_2Al are formed at the Au-Al interface, which have been reported in some published literatures [5][6][7]. Besides, the cross-sectioned samples for the experimental study are fully assembled ones, which mean that the multiple intermetallic layers should grow up more or less after undergoing 5 hours annealing process at 175°C during molding and PMC processes. This is why the “gray” intermetallic layer ranging from 0.3 - 1.0um is clearly observed between the Au bump and the Al metallization.

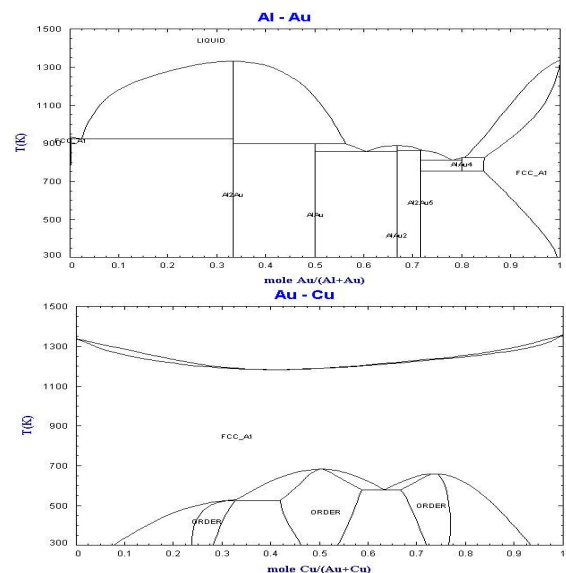


Fig.7 Equilibrium phase diagram of Au-Au (top) and Au-Cu (bottom).

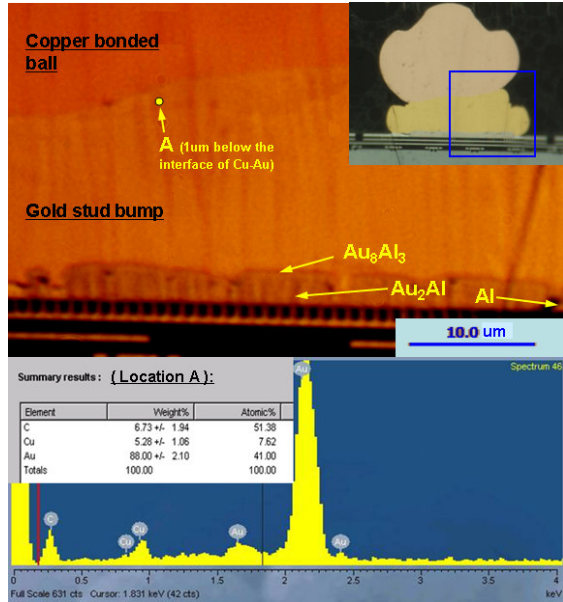


Fig.8 Images of EDS on the sectioned fully assembled sample

In contrast, mismatch of atomic radii in the Cu-Au couple reaches 11.1%. This leads to the strain energy that hinders atomic inter-diffusion at the interface of the Cu-Au couple, so atomic inter-diffusion in the Cu-Au couple is much harder and slower than that in the Au-Al couple for sure. Referring to Cu-Au equilibrium phase diagram shown in Fig.7, it reveals that Au and Cu are completely miscible in the solid state and have substitutional solid solution. Furthermore, Cu and Au have same valence and small electronegativity difference (Au vs. Cu: 2.54 vs. 1.9). Thus, when undergoing inter-diffusion of Au in Cu and Cu in Au, the solute atoms substitute the solvent atoms in the crystal lattice without structural change. Although Cu is diffused into Au with heat (at 200°C) and pressure during wire bonding, this diffusion only results in a random distribution of Cu atoms into the Au (fcc) structure and there is no atomically ordered arrangement happened in the crystal lattice. As a result, intermetallic compound products at the interface of the Cu-Au couple can not be formed on as-bonded samples even with atomic inter-diffusion. This is in accordance with the actual observation. Fig.8 shows the result of EDS analysis at the region close to the Cu-Au bonding boundary. Cu was clearly detected at the region close to the Cu-Au interface on Au bump, so it definitely indicates that atomic inter-diffusion of the Cu-Au couples happened during wire bonding process.

Growth of IMCs and Void Generation: Fig.9a shows a typical cross-sectioned image of the experimental

sample that has undergone HTB for 1008 hrs. Fig.9b shows an OM image of a cross-sectioned sample having finished TC for 1000 cycles. The two images show a fast Au-Al IMC growth and some kirkendall voids occurred as well. But at the interface of Cu-Au couple, no significant change was observed compared with the sectioned image of the as-bonded samples.

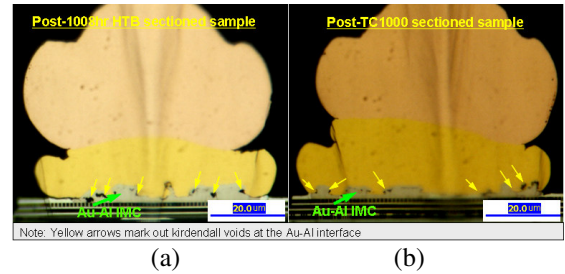


Fig.9 Images of the sectioned samples (a) post-1008hr HTB and (b) post-TC1000cycle.

IMC growth is the result of inter-diffusion of one material into another via crystal vacancies usually made available by defects, contamination, impurities, mechanical stress and temperature. Temperature can significantly accelerate the IMC growth as a critical factor. Thus, both high temperature storage and temperature cycle (HTB-1008hours and TC-1000cycles) are commonly employed to accelerate the IMC growth to investigate the wire bonding reliability. Atomic self-diffusion activation energy Q is generally defined as the sum of vacancy formation energy E_f and the vacancy migration energy E_m

$$Q = E_f + E_m.$$

For E_m , there is a relation as $E_m = E_s - E_i$ where E_i is the total potential energy of the system when there is one vacancy created at certain lattice position in otherwise a perfect crystal and theoretically $E_i = -E_f$, and E_s is the total potential energy of the system when one of the nearest neighbor atoms of the vacancy jumps to the saddle point configuration [8]. Table 1 shows the value of atomic self-diffusion energy Q .

Table.1 Self-diffusion activation energies for some cubic metals

Metals	E_f (ev)	E_s (ev)	E_m (ev)	$Q=E_f + E_m$
Cu	1.1699	-0.1606	1.0093	2.1791
Au	0.9797	+1.3401	2.3198	3.2998
Al	0.7498	+0.0498	0.7997	1.5495

In the Au-Al IMC, the atomic inter-diffusion rate is quite active due to similar atomic radii and large difference in electronegativity, where the diffusion rate for Au in Al is much slower than that for Al in Au according to Au and Al diffusion activation

energy in Table1. Au-rich IMCs are the main IMC phases at most of bonding regions due to the large amount of Au relative to Al. With time and the temperature set at 150°C, the Au-Al IMC grows laterally and vertically at the interface. This Au-Al IMC growth is doomed to consume Al in Al metallization at the bonding regions. However, in some regions where no IMC phase is formed during wire bonding process, there is no development of IMC in vertical direction. This may produce an unbalance effect on atomic diffusion along grain boundary in spatial content. When a great many of vacancy concentrations occur at a point, this inclines to become a Kirkendall void. As shown in Fig.10, Kirkendall voids have appeared after both 504hrs HTB and 500cycle TC, and Kirkendall void size is becoming larger after undergoing 1008 hrs HTB and 1000 cycles TC shown in Fig.9. From the view point of packaging quality, Kirkendall voids may accelerate deterioration of the bonding force and even ball lift from pad. But, the generation and growth of the Kirkendall voids can be improved in practice by achieving a good and even Au-Al IMC coverage on Al bond pad in as-bonded samples.

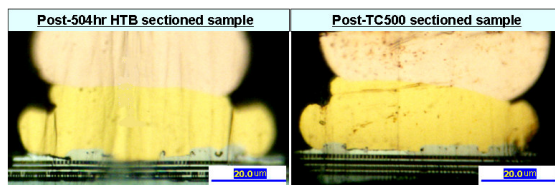


Fig.10 Images of the sectioned samples (a) post-504hr HTB and (b) post-TC500cycle

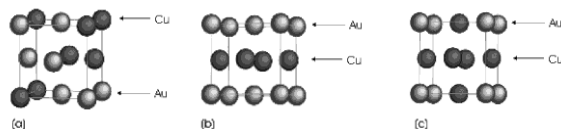


Fig.11 Diagrammatic sketch of Cu-Au cubic crystal structures (a) disordered CuAu (b) ordered CuAu and (c) ordered Cu_3Au

For the Cu-Au couple, Cu and Au have the same lattice structure and are subjected to a complete solid solubility within all composition ranges. Diffusion rate of Cu in Au is much faster than that of Au in Cu. In addition, Cu has smaller atom size than Au and Cu diffuses to Au when a temperature at the Cu-Au interface rises. At a temperature of 150°C, diffusion of Cu into Au starts from atomically disordered solid solution first. With time and temperature going up, the Cu and Au atoms gradually order into a new arrangement and the ordered solid solution at the interface of the Cu-Au couple then form a new phase,

the Cu-Au IMC. Fig.11 shows three types of Cu-Au cubic crystal structure, disordered CuAu, ordered CuAu and ordered Cu_3Au . The newly formed IMC layer generally comprises the CuAu and Cu_3Au and Cu_3Au is close to the side of Cu bonded ball due to Cu enrichment [9]. Pure Cu has a reddish brown color, pure Au has an orange-yellow color, and Cu-Au alloy has yellow color with reddish tint. Therefore, it is difficult to identify the Cu-Au IMCs existence by color within such a thin Cu-Au alloy layer. This IMC layer, however, is still very thin even after HTB for 1008hrs and TC for 1000cycles.

4. Conclusions

The formation and growth of intermetallic compounds in Cu-Au and Au-Al systems with the COG bonding have been experimentally investigated. The following conclusions are drawn:

1) COG bonding can be successfully implemented in current wire bonder with an add-on system-copper kit. A qualified and stable wire bonding on bond pads is shown and no any damage to underlying metals of bond pads occurs.

2) Compared with Au wire bonding, a comparable Au-Al IMC formation and growth is shown in the COG bonding. The Au-Al IMC formation and bonding force between Au bump and Al metallization are mainly related to bonding parameter setting for Au bump.

3) For Cu-Au couple, no clear IMC formation is observed after assembling and then much slower and thinner Cu-Au IMC appears after 1008hrs HTB at 175°C. Such slowly growing thin IMC is not sufficient to degrade mechanical performance of the Cu-Au interface.

4) Both appropriate FEO parameter setting and bonding parameter setting for Cu ball can significantly reduce opportunity of underlying metal crack and crater by minimizing yield force of Cu balls.

The above results indicates that COG bonding process can be applied to large-scale integrated circuit devices as a practicable approach with qualified package performance.

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