Role of intermetallics on the mechanical fatigue behavior of Cu-Al ball bond interfaces

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Abstract

The mechanical fatigue behavior of Cu-Al interfaces occurring in thermosonic ball bonds – typically used in microelectronic packages for automotive applications – is investigated by means of a specially designed fatigue test technique. Fully reversed cyclic shear stresses are induced at the bond interface, leading to subsequent fatigue lift off failure and revealing the weakest site of the bond. A special focus is set on the role of interfacial intermetallic compounds (IMC) on the fatigue performance of such interfaces. Therefore fatigue life curves were obtained for three representative microstructural states: The as-bonded state is compared to two annealed states at 200 °C for 200 h and at 200 °C for 2000 h respectively. In the moderately annealed state two IMC layers (Al_2Cu , Al_4Cu_9) could be identified, whereas in the highly aged state the original pad metallization was almost entirely consumed and AlCu is formed as a third IMC. Finally, the crack path is traced back as a function

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of interfacial microstructure by means of electron microscopy techniques. Whereas conventional static shear tests reveal no significant decrease of the bond shear force with increased IMC formation the fatigue tests prove a clear degradation in the cyclic mechanical performance. It can be concluded that during cycling the crack deflects easily into the formed intermetallics, leading to early failure of the ball bonds due to their brittle nature.

Keywords: Cu-Al ball bond, microelectronics, intermetallic compound formation, bonding interface, high cycle fatigue, automotive applications

1. Introduction

In the past decade thermosonic ball bonding has become a key technology for microelectronics devices to create electrical connections between integrated circuits and their external circuitry [1]. Recently, Al pad and Cu bonds have become a state of the art materials combination. The reliability of bonding interfaces has gained a lot of attention since they dictate the overall quality of microelectronic devices, which become more and more indispensable in our every day lives. Principal achievements in Cu wire bonding are summarized in a review by Schneider-Ramelov et al in [2]. During service conditions microelectronic devices are subjected to elevated temperatures of up to 150 °C for about 10000 service hours. In the case of wire bonded interfaces, significant microstructural changes impairing the bond properties are expected. For bimetallic bonds, intermetallic compound (IMC) formation occurs as a consequence of marked interdiffusion of both materials into each other [3, 4]. Compared to their soft and ductile parent materials, Al-Cu intermetallics highly differ in their physical properties: volumetric shrinkage,

increased hardness and brittleness [5] highly affect the performance and reliability of such interconnects [6]. Moreover, increased resistivity of one order of magnitude leads to further local Joule heating, which additionally fosters interdiffusion among the materials involved. Kouters et al. [7] characterized the physical properties of the intermetallics, where a special focus is set on their mechanical behavior: Al-Cu intermetallics feature increased hardness of more than one order of magnitude than the original bonding materials. Indentation fracture toughness of intermetallics, which are almost two orders of magnitude lower than their ductile parent materials indicate that these intermetallics will fail in a brittle way. Physical properties of intermetallics formed below 300 °C are summarized in table 1. In light of this, IMC formation is usually associated with an overall bond degradation but their impact on bond reliability and impairment is not yet fully understood.

Several studies [8, 9] compared intermetallics formation in Al-Cu bonds with formerly used Au-Al bonds by means of isothermal heat treatments. Both material combinations revealed a parabolic relationship of the growth of IMC as a function of annealing time. Al-Cu interdiffusion kinetics occur 10 times slower than Al-Au, which is one of several benefits of the established Al-Cu combination. The delayed Al movement in Cu may be attributed to their 10.5 % atomic misfit, whereas the atomic radii of Al and Au are very similar. Lower chemical activity of Al-Cu vs. Al-Au IMC formation is explained by one of the Hume Rothery Rules stating that the higher the difference of electronegativity of both materials, the more chemical activity between both is favored. For Au, Cu, Al electronegativities are 2.54, 1.9 and 1.61 eV respectively. Previous studies stated that in the as-bonded condition no traces

of Al-Cu intermetallics could be found, whereas Drozdov et al. identified Al_2Cu nuclei in the very initial state [10]. Therefore, it may be concluded that the as-bonded microstructure highly depends on the bonding parameters as well as on the surface condition of the parts to be bonded. Xu et al. [4] found that the first intermetallic compound is Al_2Cu , followed by Al_4Cu_9 . In the same study various intermetallics were discussed, where it is shown that polymorphism in the Al-Cu system exists. Additionally, once the Al pad material has been entirely consumed a second reaction occurs where Al_2Cu is transformed into Al_4Cu_9 differing in its crystal structure from the primarily formed Al_4Cu_9 . On the other hand Hang et al. [11] and Pelzer et al. [12] identified a third IMC, possibly AlCu . Various studies compared the effect of interfacial evolution on the mechanical properties of ball bond interfaces by means of standard destructive shear tests. E.g. Pelzer et al. [13] have thoroughly characterized Cu-Al ball bond shear strengths as a function of heat treatments: It was found that the activation energy for the entire intermetallic stack is 1.26 eV. Static shear values were compared to the annealing matrix but significant changes in the shear force values with increased IMC formation was not observed. In another study, Amistoso et al. [15] found a slight decrease of ball shear strength as a function of time and temperature. Bond degradation due to intermetallics formation has usually been associated to the formation of cracks and voids subsequent to interdiffusion and not to the intrinsic physical properties of the intermetallics. Currently, state of the art test techniques to evaluate the bond quality are the above mentioned static shear and wire pull tests. Both do not reveal the bond performance under cyclic loads and thus fatigue properties are still

unknown due to a lack of suitable test methods. Albeit, it is well known that fatigue of structural components is still the main failure cause in engineering applications. In the case of wire bonds, interfaces are subjected to cyclic loads due to mechanical and thermomechanically induced stresses. Therefore it is crucial to assess the bond quality taking cyclic stresses into account. Recently a novel fatigue test technique for thick Al wedge bonds has been introduced by Khatibi et al. [16]. Utilizing an ultrasonic resonance fatigue system in combination with a special specimen setup cyclic fully reversed shear stresses are induced in the bond interface, revealing the weakest site. In this work an improved fatigue test setup specially designed to study the fatigue properties of miniaturized ball bonds is presented, basing on previous prototypes [17], [18]. Three fatigue life curves are measured, where a special emphasis is set on the role of intermetallic compound formation. The following representative microstructural states are chosen: as-bonded, a moderately annealed (200 °C, 200 h) and highly aged state (200 °C, 2000 h), revealing different intermetallic compound layers. Finally, typical fatigue fracture morphologies were analyzed by means of electron microscopy and FIB techniques.

2. Methods and Materials

2.1. Investigated Specimens and High Temperature Storage

The investigated specimens are thermosonic Cu-Al ball bonds, which are typically used as first bond interconnects for automotive applications. A 50 μm thick Cu wire of 99.99 % purity is bonded on a 5 μm sputter deposited Al pad metallization. For the bond process a state of the art ASM

Table 1: Physical properties of Al-Cu intermetallic compounds [7].

Material	at.%Cu	E (GPa)	ρ g/cm ³	K _{1C} MPam ^{1/2}	HV MPa	form. E eV/atom	CTE ppm	Crystal structure
Al	0-2.84	70	2.7	14-28	20-50		23.5	fcc
Al ₂ Cu	32-33	124 ± 7	4.38	0.27 ± 0.06	324	-0.1553	16.1	tetragonal
AlCu	50-52	180 ± 13	5.36	0.20 ± 0.03	628	-0.2134	11.9	monoclinic
Al ₃ Cu ₄	55-56	na	na	0.21 ± 0.05	616		16.1	monoclinic
Al ₂ Cu ₃	59-62	na	na	0.68 ± 0.15	558		15.1	trigonal
Al ₄ Cu ₉	63-69	187 ± 9	6.85	0.67 ± 0.10	549	-0.2105	17.6	cubic
Cu	80-100	120	8.93	12-22	60-100		17.3	fcc

iHawk Xtreme bonder equipped with a reducing atmosphere nozzle was employed. As a reducing atmosphere the mixture of gases N₂ – H₂ was employed with a concentration of 95% : 5%, respectively, which was limited by security reasons. The resulting bond has a diameter of approximately 135 μ m. The deformed Cu ball height is about 30 μ m high.

Three representative microstructural states for the bonding interface were chosen: (i) as-bonded (ii) intermediately aged, where thin IMC layers are already formed and (iii) highly aged. In state (iii) a pronounced interfacial evolution is observed, where the IMC formation has almost entirely consumed the pad metallization. State (ii) and (iii) were achieved by isothermal heat treatments under vacuum at 200 °C after 200 h and 2000 h respectively. In Fig. 1 a SEM cross section of the ball bond is shown indicating a throughout and parallel interface across the bond. Furthermore, a pronounced splash of the pad can be observed in the bond periphery due to the high plastic

Figure 1: SEM Cross section of investigated ball bond specimen with close-up of interfacial evolution of three investigated states (a) as-bonded state (b) 200 °C, 200 h (c) 200 °C, 2000 h.

deformation caused by the bond process. Pad squeeze out is usually observed if the pad material is relatively softer than the wire material. Here, the bonding process was adjusted to ensure a residual pad thickness of 2-2.5 μm below the Cu ball. A close up of the three investigated microstructures obtained by scanning electron microscopy are shown in Fig. 1a, b and c. In the as-bonded state no intermetallic compounds are visible, whereas in the moderately aged (200 °C, 200 h) state a total stack of 1.4 μm consisting of two thin intermetallic layers is visible. In the highly aged state (200 °C, 2000 h) the Al pad is almost entirely consumed. Furthermore three intermetallic compounds can be found, which form an entire IMC stack of up to 3.9 μm thickness. To characterize the individual IMC layers an electron transparent lamella was extracted by focused ion beam (FIB) from the highly aged bond interface (200 °C, 2000 h) and analyzed using a scanning transmission electron microscope (STEM) operating at 300 kV equipped with a Bruker

Figure 2: Elemental map of highly aged (200 °C, 2000 h) Cu-Al ball bond interface: a) HAADF image b) color-coded Cu distribution map revealing 5 distinct materials: aluminum (1), Al-Cu intermetallic compounds (2-4) and Cu (5); see Tab. 2 for detailed analyses.

four quadrant energy dispersive X-ray spectroscopy (EDX) detector. Fig. 2a shows a high angle annular dark field (HAADF)-STEM image revealing five different material layers. Fig. 2b shows a color-coded map of the elemental distribution of copper. The measured atomic % of Cu in each layer is summarized in Tab. 2. The atomic percentage nicely coincides with the literature data in Tab. 1. The intermetallic compounds can thus be identified as Al_2Cu , AlCu and Al_4Cu_9 . For the intermediately aged state (200 °C, 200 h) it is well-known from [13] that only Al_2Cu and Al_4Cu_9 are present.

2.2. Static shear test of Cu-Al interface

Standard shear tests were conducted on heat treated samples at 200 °C from 0 h (i.e. as-bonded) up to 2000 h to compare the effect of intermetallics evo-

Table 2: Quantitative TEM-EDX map results of highly aged (200 °C, 2000 h) Cu-Al bond interface. For the corresponding region compare with Fig. 2.

region	Cu	Cu	material
	measured at. %	comp. lit. ^[7] at. %	
1	3	0-2.84	aluminum
2	35	32-33	Al ₂ Cu
3	50	50-52	AlCu
4	67	63-69	Al ₄ Cu ₉
5	96	80-100	copper

lution on the static shear strength of the bond. For these tests a standard XYZTCondor100 ball shear tester was used. The adjusted ball shear tool was positioned 5 μm above the pad. The shear force required to rupture the bond is plotted against the duration of storage and summarized in Fig. 3, where the mean value and corresponding 3 sigma confidence is given. For each measurement series approximately 20 bonds were tested. Considering the standard deviation for the obtained shear values, no significant bond degradation as a consequence of high temperature storage up to 200 h can be seen. However, a slight increase of the shear strength is noted at the heat treatment at 200 °C for 250 h resulting from the formation of hard inter-metallics. At high annealing durations of 1000 h and 2000 h at the same temperature, a significant decrease of the ball shear test is noted.

2.3. Fatigue tests of the Cu-Al bond interface

To study the fatigue behavior of miniaturized ball bond interfaces, an accelerated fatigue test basing on the functional principle described in [16] was specially modified. The main steps of this test technique are briefly explained hereafter. The setup consists of an ultrasonic resonance fatigue

Figure 3: Shear test results as a function of isothermal annealing at 200 °C.

setup, where each component including the sample holder fulfills the resonance condition at 20 kHz. Consequently, strain and displacement signals follow a sine-shaped standing wave along the setup during longitudinal push-pull excitation. The testing device is mounted at the end of the specimen holder (i.e. at the location of maximum acceleration) such that the testing interface acts as a coupling joint between two differently inert masses: the bulk sample holder and the active mass above the bond. Differently inert masses lead to a slightly phase shifted motion resulting in cyclic shear stresses at the bond interface, leading to subsequent lift off failure, where the micro component is detached at the fatigued bond interface. The average cyclic shear stress amplitude τ acting on the bond during the fatigue test can be estimated by equation 1.

$$\tau = (m \cdot a)/A \quad (1)$$

with m denoting the active mass above the bond, a the acceleration of the setup and A the bonding area, which is measured post mortem. It can be deduced from equation 1 that a suitable mass-to-area-ratio is required to obtain sufficiently high shear stresses leading to fatigue failure. In the case of miniaturized, loaf shaped ball bonds, a special sample preparation is required to increase the mass of the ball artificially. A laser assisted solder jetting method is chosen, where solder bumps can be precisely positioned with a capillary tool. An ultrafast laser pulse is used to reflow the eutectic PbSn solder sphere of 400 μm diameter, which is placed onto the Cu ball. Therefore a solder jetting device SB²-M from PacTech was used. The sample preparation method is briefly sketched in Fig. 4. Prior to soldering, the wire is carefully removed followed by a surface cleaning procedure with ethanol

Figure 4: Key steps for solder jetting of fatigue specimen

ensuring impeccable adhesion between the solder sphere and the Cu bump. Finally, the prepared fatigue specimen is glued at the end of the bar shaped sample holder as shown in Fig. 5. Finite element analyses of the loading conditions occurring at the bond interface during fatigue loading are presented elsewhere in [14].

In this study three lifetime curves of the sample with the selected microstructures described in 2.1 were measured by means of above mentioned fatigue testing setup. The applied stress amplitude was determined according to equation 1, where the acceleration was obtained by strain measurements with a strain gage mounted at the strain node of the load train, as described in [16]. The active mass and the bond-area were measured post-mortem. The fatigue experiment was monitored with a camera to determine the number of loading cycles to failure to catch the time step, where the fatigue lift-off occurs. Typical micrographs of the selected microstructures are presented hereafter in Fig. 1.

Figure 5: Scheme of fatigue set-up: Position of micro-component on the sample holder (a) close-up cyclically loaded specimen (b) fatigue lift-off at weakest site of interface(c)

3. Results and Discussion

3.1. Fatigue results

The S-N data is summarized hereafter in Fig. 6, where the average shear stress amplitude according to equation 1 is plotted as a function of loading cycles to failure N_f . In the as-bonded state the fatigue data ranges from about 14 MPa to 11 MPa along 10^5 to 10^8 loading cycles. Runouts- i.e. bond specimens without fatigue failure up to 10^9 loading cycles- were observed at 9 MPa. In the as-bonded state, the fatigue limit is reached at stress amplitudes below 10 MPa, whereas in the slightly aged state (200 °C, 200 h) the fatigue data ranges between 12 MPa and 8 MPa. It has to be noted that in this state no run outs were observed. In the highly aged state (200 °C, 2000 h) the data is significantly lower and ranges between 10 MPa and 6 MPa, which corresponds to a drastic reduction of fatigue reliability compared to the as-bonded state. The fatigue tests were conducted such that the loading

Figure 6: Lifetime curves of Cu-Al ball bonds: applied shear stress $\Delta\tau$ vs. loading cycles to failure N_f . The dashed lines serve as guide for the eye for each microstructural state.

direction (the longitudinal to and fro motion) of the ultrasonic fatigue setup is parallel to the thermosonic ball bonding direction (visible by the aluminum splash) of all the investigated bond samples.

3.2. Fatigue fracture morphology

An overview of typical fatigue lift off fractographs of the investigated microstructures is depicted in Fig. 7, showing the fatigue surface of the bond pads (Fig. 7a-c) and the corresponding separated interface on the Cu ball bonds (7d-f). Each image is oriented parallel to the loading direction (LD),

which also coincides with the bonding direction. In all three states two different fracture morphologies can be identified and related to characteristic failure which are: (i) crack propagation and (ii) final fracture: The given bond geometry forces crack initiation at the bond periphery as the (unbonded) notch shaped gap between the Al splash and the Cu ball acts as a stress concentrator (see Fig. 1). During cycling, the crack propagates symmetrically from the bond periphery inwards until only a small area remains bonded. Consequently, the resulting stresses according to equation 1 become significantly high due to area reduction, which leads to final -abrupt- fracture. The ultimate fracture regime is characterized by the elliptical feature in the center of the bond, where the short dimension of the ellipse is parallel to bond and load direction. This regime highly differs in its morphology compared to the crack propagation regime and occurred in a different material. Both fracture regimes were observed in the three investigated conditions however the crack path differed depending on the formed intermetallic compounds as well as on the thickness of residual aluminum pad. In the as-bonded state, where only the soft and ductile parent materials constitute the bonding interface, crack propagation occurs within the soft Al metallization, whereas final fracture occurs at the bond interface as confirmed by the fractographs of the separated bonding surface in Fig. 7a, b. The crack propagation regime is denoted by marked striations which are formed parallel to the propagation direction, final fracture is characterized by ductile dimples. For the aged specimens SEM-EDX maps of representative fatigued pads were obtained to identify the phases involved in the fracture path, see Fig. 8. The data is summarized in table 3. A discrepancy between the measured at. %

of Cu compared to literature values in 1 can be explained by the underlying aluminum rich material layers leading to an underestimation of the Cu at. %. In the case of slightly annealed samples (200 °C, 200 h) the crack propagation stage occurs in the soft Al pad, since this is the softest material, which is easiest to deform. Crack path deflection in both- as-bonded and slightly annealed states- is similar and is mainly enhanced due to a tilting component during the fatigue test (as previously described in [17]). It can be assumed that since sufficient Al metallization remains in both conditions, a similar fatigue performance depending on the selected method can be explained. However, in the highly aged state crack propagation occurred in two different materials due to irregular aluminum consumption. Thus, if Al metallization is still present, crack growth occurs through the soft material, in regions, where Al has been entirely consumed and intermetallics are fully developed, crack is kinked into Cu for further crack growth. Final fracture could be identified in the third intermetallic AlCu, which is hardest but also least tough material. Since the crack propagation in the highly aged state cannot be predicted in a straightforward way, it follows that the underlying microstructure needs to be taken into account to understand possible crack deflections. Therefore FIB cross-sections were realized parallel to the loading direction along the fatigued pad to correlate the EDX measurements and the underlying microstructural evolution with the surface fracture morphologies of the fatigued specimens. Fig. 9 confirms previously gained assumptions about the preferential crack paths. Fatigue fracture paths as a function of the microstructural evolution are sketched and summarized in Fig. 10.

Figure 7: SEM fatigue fracture surfaces revealing the bonding pad (top) and corresponding Cu ball (bottom) for each microstructural state: (a)-(d) as-bonded, (b)-(e) 200 °C, 200 h, (c)-(f) 200 °C, 2000 h. The crack propagation zones and final fracture areas are denoted by (i) and (ii), respectively and will be further discussed in Fig. 9.

Figure 8: EDX maps of fracture surfaces of the bonding pad in the annealed states: (a-b) correspond to 200 °C, 200 h and (c-d) correspond to 200 °C, 2000 h. Left at. % Al and right at. % Cu

Figure 9: FIB cross sections parallel to the bond and load direction (LD) revealing the two states (i) crack propagation (ii) final fracture characteristic for each microstructure. (a) as-bonded: (i) in Al and (ii) in Al pad; (b) 200 °C, 200 h: (i) in Al and (ii) at the interface between Cu and Al_4Cu_9 ; (c): (ia) in Al followed by crack deflection (ib) at the the interface between Cu and Al_4Cu_9 (ii) AlCu.

Table 3: Summary of EDX results of crack path: (ia) crack propagation (ib) crack deflection (ii) final fracture

	200 °C, 200 h	200 °C, 2000 h
	Material (at.% Cu)	Material (at.% Cu)
stage (ia)	Al (1 at.% Cu)	Al (1 at.% Cu)
stage (ib)	-	Al_4Cu_9 (56 at.% Cu)
stage (ii)	Al_2Cu (24 at.% Cu)	AlCu (46 at.% Cu)

Figure 10: Typical fracture of (a) as-bonded (b) 200 °C, 200 h (c) 200 °C, 2000 h state. In (a) crack propagation (i) occurs in the soft Al until final fracture (ii) occurs at the original Al-Cu bond interface. (b) crack propagation (i) occurs in the Al pad final fracture occurs (ii) at the interface between both intermetallics Al_2Cu and Al_4Cu_9 in (c) crack propagation occurs in Al (ia) once Al is entirely consumed it is deflected into the interface between Cu and Al_4Cu_9 (ib) final fracture occurs in AlCu

4. Summary

This paper presents a novel approach to assess high cycle fatigue properties ($10^5 < N_f < 10^9$) of bimetallic miniaturized bond interfaces. Therefore a new test technique is specially designed for miniaturized ball bonds and is based on inducing cyclic shear stresses at the bond interface. In contrast to standardized static test techniques this method is particularly sensitive to interfacial evolution like intermetallic compound formation and reveals the weakest link in a bonding interface.

Whereas ball shear tests do not represent the application relevant loading

conditions and impact of interfacial evolution on the reliability of a bond, fatigue tests proved a clear degradation with increased intermetallics formation. Characteristic fracture morphologies revealed that due to the given geometry and presence of the sharp notch of the bond periphery (cf. Fig. 1 two stages occur during fatigue failure: (i) crack propagation and (ii) final fracture. The crack path highly depends on the microstructural evolution of the bond. However, in final fracture or when the pad material is entirely consumed, interfacial intermetallics are responsible for failure. In this study three characteristic interfacial states were investigated as a function of interfacial evolution. With the presented fatigue test technique the typical crack paths are summarized and schematically shown in Fig. 10. By comparing the physical properties of each individual intermetallic compound in table 1 AlCu is the hardest material but also features the lowest fracture toughness, resulting in a crack deflection into this material since Al does not entirely act as a buffer material during cyclic loading of the highly aged samples.

as-bonded: (i) crack propagation in Al pad (ii) final fracture at the original Al-Cu bond interface

200 °C, 200 h: (i) crack propagation in Al pad (ii) final fracture at the interface between Al_2Cu and Al_4Cu_9

200 °C, 2000 h: (ia) crack propagation in remaining Al and deflection (ii) at the interface between Cu and Al_4Cu_9 (ii) final fracture in AlCu

It is shown that the crack propagates through the Al pad material, final fracture however occurs in the most brittle site. This study reveals that lifetime of Cu-Al bonds is directly related to the amount of residual aluminum

pad metallization.

For the reliability of the investigated Al-Cu ball bond interface it may be concluded that it is crucial to ensure a throughout, residual aluminum layer below the evolved intermetallic compounds. At this point it should also be noted that according to the study of Pelzer et al. [13] annealing treatments conducted at 200 °C correspond to the 39-fold annealing durations conducted at 150 °C. The manufacturer guarantees reliable bonds annealed at 150 °C up to 10 000 h, this microstructural end of life state corresponds to an annealing treatment at 200 °C for 256 h.

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