

Simulation of Diffusion Controlled Intermetallic Formation of Au/Al Interface

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Abstract

This paper describes the finite element simulation for diffusion controlled intermetallic formation of Au/Al interface during the wire bonding process. The analogous correlation between the intermetallic atomic diffusion and the heat transport is introduced, and the simulation of intermetallic diffusion using a commercial finite element method (FEM) tool ANSYS is demonstrated. Phase dependent diffusivities have been implemented into the material model in order to more accurately model the distribution of diffusing atomic concentration. The various phases of intermetallic compounds (IMCs) can be determined briefly by the obtained atomic concentration profile from FEM and the phase composition table. The overall thickness of the IMCs layer can then be calculated. In this paper, the concept for the subsequent stress analysis based on the volume change due to diffusion is also discussed.

1. Introduction

Wire bonding is the primary method in packaging technologies to make the interconnection between a semiconductor device and a printed circuit board (PCB). About 90% of the total microelectronics packaging is fabricated using wire bonding technique. The most commonly used process is thermosonic bonding of high purity Au 99.99% (4N) wires to Al pads. During the wire bonding process, the combined mechanical, ultrasonic and thermal energies are employed to form the bonds.

Previous studies showed that different intermetallic compounds (IMCs) may form at Au/Al interface at elevated temperatures during the wire bonding process and as well as the subsequent packaging processes such as molding, post mold cure, and annealing after plating. Under such conditions intermetallics can grow due to thermally activated reactive diffusion [1-4]. The growth of intermetallics usually exist in the form of five phases: AuAl₂, AuAl, Au₂Al, Au₅Al₂ (Au₈Al₃), and Au₄Al. Such IMCs are associated with Kirkendall voids, detrimentally affecting the reliability of devices [5, 6]. IMCs growth and potential formation of voids and cracks have a significant impact on the strength and reliability of bonds. If IMCs are formed in a proper amount at the wire bond interface, it enhances the bond contact. However, the excessive growth of IMCs can lead to the bond interface degradation which results in greater brittleness, contact

resistance, and heat generation. Therefore, intermetallic growth and subsequent void formation in some particular phase such as Au₄Al can dramatically weaken the bond which impairs the reliability of devices and leads to electrical failure.

IMCs formation has been intensively studied both for the Au/Al and Cu/Al interface system. There have been many publications with respect to experimental investigations in order to observe the morphology and composition, to evaluate the thermodynamic driving force, to determine the activation energy and diffusion constant, and to analyze the kinetics and mechanism of the IMCs formation [1-4, 6-12]. However, the modeling and simulation regarding the IMCs formation of either Au/Al or Cu/Al are seldom reported to our best knowledge. Still most of the work is focused on theoretical modeling of diffusional phase transformation in binary or multiple component systems with stoichiometric phase [13-16]. An engineering tool called DICTRA for diffusion simulation in multicomponent alloys has been developed. In the above cases, thermodynamic and kinetic data such as phase formation energies and diffusion coefficients are necessary to be supplied by experiments or other means. Recently modeling IMCs growth has been performed by Ulrich [8], that a phenomenological model describing the reaction kinetics can be built up from the quantum-mechanical density functional theory (DFT) and tracer diffusion coefficient calculation based on atomic diffusion theory. However, all the aforementioned approaches can only be applied for one-dimensional geometries. The extension and application of the models are rather complicated. Besides that, some of them require the specific modeling procedure for acquiring parameters of certain IMCs formation.

In this study, we attempted to explore a relatively simpler way to predict the IMC's formation, by using commercial FEM tool ANSYS. By means of the analogue of transient thermal analysis, the diffusion controlled IMCs formation can be simulated. The general approach, the obtained results, the discussions, and the possible approach for subsequent stress analysis are presented.

2. Simulation Approach

2.1 The Analogue to Thermal Analysis

During IMC formation, intermetallic diffusion which is driven by atomic concentration gradient, can be described by the second Fick's law as follows (e.g. in one-dimensional case):

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \quad (1)$$

where C represents the concentration of the diffused atom, D refers to the diffusion coefficient, t is the time, and x is the location.

The fundamentals of three-dimensional heat flow which is used in ANSYS can be presented as equation (2) if only considering heat conduction and convection. Temperature gradient acts as the driving force of heat flow.

$$\rho c \left(\frac{\partial T}{\partial t} + V_x \frac{\partial T}{\partial x} + V_y \frac{\partial T}{\partial y} + V_z \frac{\partial T}{\partial z} \right) = k_x \frac{\partial^2 T}{\partial x^2} + k_y \frac{\partial^2 T}{\partial y^2} + k_z \frac{\partial^2 T}{\partial z^2} + \dot{q} \quad (2)$$

where ρ is the density, c is the specific heat, T is the temperature, v is the convection velocity, t is the time, x , y , z represents the location in the global Cartesian system, k is thermal conductivity, \dot{q} is the heat generation rate per unit volume.

In analog with diffusion process, only the conduction part is available and thus the convection part can be neglected. Thus, equation 2 can be simplified to

$$\rho c \left(\frac{\partial T}{\partial t} \right) = k_x \frac{\partial^2 T}{\partial x^2} + k_y \frac{\partial^2 T}{\partial y^2} + k_z \frac{\partial^2 T}{\partial z^2} + \dot{q} \quad (3)$$

Furthermore, if only considering a closed system in one-dimensional case which means there is no heat source, equation (3) can be further simplified to

$$\rho c \left(\frac{\partial T}{\partial t} \right) = k \frac{\partial^2 T}{\partial x^2} \quad (4)$$

Now if we compare equation (4) with equation (1). A correspondence of parameters in both equations between transient thermal analysis and diffusion analysis can be summarized in Table 1.

Table 1: Analogous comparison between thermal and diffusion analysis

Thermal analysis			Diffusion analysis		
Symbol	Description	Units	Symbol	Description	Unit
T	Temperature	K	C	Normalized Atomic concentration	/
t	Time	S	t	Time	s
k	Thermal conductivity	W/mK (J/m K s)	D	Diffusivity	$\mu\text{m}^2/\text{s}$
ρ	Density	kg/m^3	ρ	Density	$\mu\text{g}/\mu\text{m}^3$
c	Specific heat capacity	J/kg K	c	No physical meaning	/

Though the density ρ can be used physically as the same, the specific heat capacity c has no true physical meaning in atomic diffusion analysis. Nevertheless, if we set $\rho c = 1$ which means $c = 1/\rho$, the temperature T and

thermal conductivity k can be directly corresponded to the atomic concentration C and the diffusivity D , respectively.

2.2 Diffusion Controlled IMCs Formation

In a solid state reaction analysis, the total increase of IMCs thickness Δx with respect to the aging time t can be estimated by using the parabolic law as follows [17]:

$$\Delta x = (Dt)^{1/2} \quad (5)$$

where D is growth rate constant which is equivalent to diffusivity if IMCs formation is diffusion controlled. In general, the solid state growth can follow either linear or parabolic growth kinetics. Linear growth implies that the growth rate is limited by the reaction rate at growth site. In contrast, parabolic growth indicates that the growth is controlled by atomic diffusion. Most of researches use a comprehensive diffusivity parameter for the whole IMCs layer formed at the bond interface due to the complexity to distinguish individual IMC phase and measure its thickness as they are usually non-homogenously layered against each other.

In fact, the magnitude of the growth rate constant of IMCs varies with different phases of Au/Al IMCs. It also depends on the remaining Au and Al layer whether they can still supply additional Au and/or Al atoms for continuous IMCs growth. Equation (5) is only valid for calculating the diffusivity when the thickness of individual phase increases constantly.

According to the Arrhenius equation as below, the diffusivity is determined by the activation energy Q , the diffusion coefficient D_0 , and the absolute temperature T .

$$D = D_0 \exp\left(-\frac{Q}{RT}\right) \quad (6)$$

where R is the molar gas constant. By measuring the individual IMCs thickness at various temperatures, the activation energy and diffusion coefficient of each phase can be acquired. One must note that IMCs growth rate can vary depending on the bonding materials and conditions. The inter-diffusion can be more rapid if there are more defects such as vacancies, dislocations and grain boundaries. Thus, the obtained activation energies and diffusion coefficients can vary and be very much microstructure dependent. In this study, equation (6) has been used to calculate the diffusivity of individual IMC phase based on the experimental data of activation energy and diffusion coefficient.

2.3 The Phase Dependent Diffusivities

The Au/Al system exhibits a rich phase diagram with a number of stable intermetallic phases. Those which are most relevant to wire bonding are listed in Table 2, along with their atomic compositions, activation energies and diffusion coefficients. The values of activation energy and diffusion coefficient in Table 2 were obtained from the internal "HOTCAR" project. All phases of compound in Table 2 have the same value of activation energy, which may not be accurate. These material properties will be

used as an initial analysis in the subsequent FEM modeling.

Table 2, Material data of Au/Al compounds

Compound	Composition (at. % Au)	Activation energy (eV)	Diffusion coefficient ($\mu\text{m}^2/\text{s}$)	Density (g/cm^3)
Au	84-100			19.3
Au_4Al	80-81.2	0.9	1.2×10^{-3}	16.52
Au_5Al_2	71.43	0.9	4.6	14.94
Au_2Al	65-66.7	0.9	1.8×10^{-1}	14.53
AuAl	50	0.9	1.85×10^{-3}	10.94
AuAl_2	32.92-33.92	0.9	4.0×10^{-2}	7.64
Al	0.006	0.9		2.7

2.4 Experimental Setup

In experiments, the Au/Al wire bond was made by 4N gold wire with $38\mu\text{m}$ wire diameter on $1.4\mu\text{m}$ thick Al pad metallization. Samples were thermally aged under 150°C for the time interval of 0, 168, 500 and 1000 hours. The cross sectioning process was applied in order to achieve the most accurate thickness measurement. The IMC layers were observed under Zeiss high power optical microscope at 50k times magnification and the thickness of the total IMC layer was measured. After measuring the IMC thickness, samples from thermal aging of 0, 168 and 1000 hours were chosen for IMC phase analysis. The analysis process was carried out by first cutting the Au/Al interface on the desired coordinate using focused ion beam (FIB). Energy dispersive X-ray (EDX) was then employed to detect IMC phases.

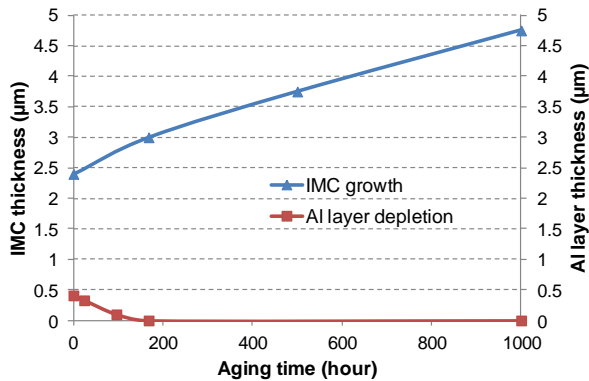


Figure 1: The overall IMC thickness evolution and Al layer depletion during IMC formation.

The total IMC thickness as well the remaining thickness of Al layer is plotted as function of aging time in Figure 1. It is shown that IMC layer increases in a sub-linear manner where the growth is proportional to the root mean square with respect to thermal aging time. IMC growth continues after 168 hours when Al layer is completely consumed. As shown in Figure 2, IMC phase transformation follows the trend of from Al-rich to Au-rich phase. At 0 hour, Al_3Au_8 exists near the Al metallization and AlAu_4 is found in between Al_3Au_8 and Au wire as shown in Figure 2(a). By thermal aging the Al_3Au_8 phase gets less as observed in Figure 2(b) and fully transformed to AlAu_4 after 1000 hours as observed in Figure 2(c).

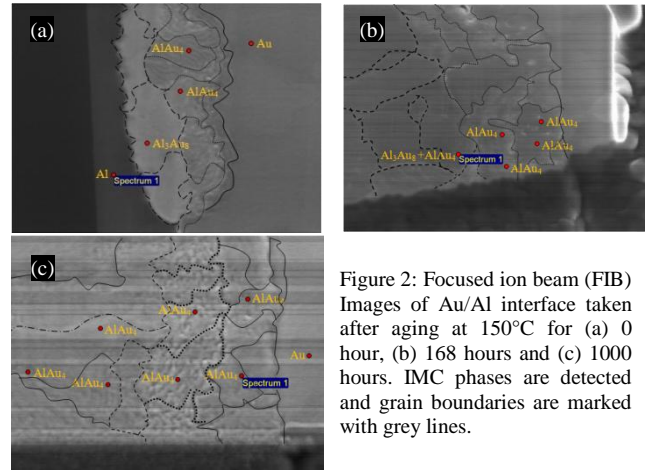


Figure 2: Focused ion beam (FIB) Images of Au/Al interface taken after aging at 150°C for (a) 0 hour, (b) 168 hours and (c) 1000 hours. IMC phases are detected and grain boundaries are marked with grey lines.

2.5 Simulation Model and Results

The simulation has been performed using commercial finite element method (FEM) tool ANSYS: A 2D model was built up based on experimental observations. The initial geometry is composed of $0.5\mu\text{m}$ Al (0% Au at.%), $1\mu\text{m}$ Au_8Al_3 (71.43% Au at.%), $1.4\mu\text{m}$ Au_4Al (80% Au at. %) and $10\mu\text{m}$ Au (100% Au at.%) sequentially from left to right, which conforms with the layer structure of FIB cut cross-section at 0 hour. Accordingly, the material properties such as diffusivity and density can be attributed to those areas. The aging temperature set in the simulation is 150°C . The diffusivity of pure Au and Al uses their atomic self-diffusivity 4.4×10^{-18} and $3.13 \times 10^{-24} \mu\text{m}^2/\text{sec}$, respectively. As it has been demonstrated by many other researches that Au atoms are the dominant diffusion species at Au/Al interface [5, 11], only Au atomic concentration is considered in the simulation. It refers in Table 2 the atomic concentrations with respect to various IMC phases. Thus, as the initial condition in the model it is set 71.43% and 80% Au for Au_8Al_3 and Au_4Al , while 0% and 100% Au for pure Al and Au, respectively. Certainly, it is defined 100% Au at the end of Au layer as the boundary condition to represent the infinite supply of Au atoms.

The direct output from the simulation is the atomic concentration of Au with respect to the location and time. As illustrated in Figure 3, atomic concentration profile of Au can be plotted along the perpendicular direction of IMC interface at any time points. Together with Table 2, the determination of total IMC thickness becomes possible: the region containing 0-84% atomic concentration of Au is the thickness of IMC compounds. The region above 84% Au atomic concentration can be determined as pure Au layer.

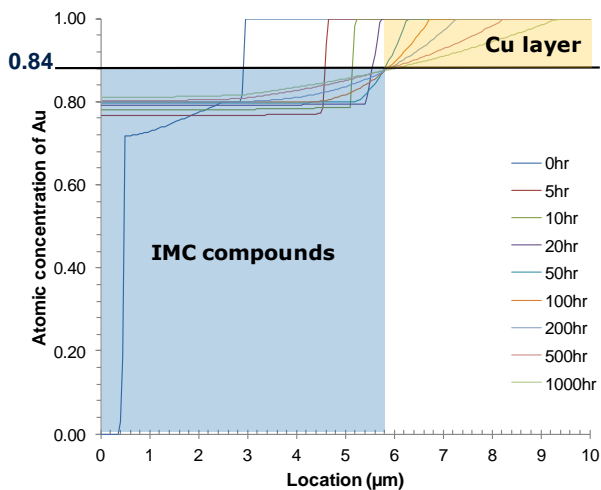


Figure 3: Diffusion profile of Au atoms at various time stages. The region above 84% Au atomic concentration can be determined as pure Cu layer. Naturally the region below 84% Au atomic concentration is the area of IMC compounds.

In Figure 4, several scenarios of the total IMC thicknesses obtained from simulation are plotted as function of thermal aging time in comparison with the experimental observation. If the diffusivity data in Table 2 is used, it is obvious to notice that the result (simulation_01) largely deviates from the experiment. In this scenario, the IMC growth is significantly faster, and the total IMC thickness is much larger. It indicates that the diffusivity data used in the simulation are far too high, especially for the Al rich phases, because the Al layer is completely consumed within the first 5 hours as shown in Figure 5. Thus, two additional scenarios are simulated (simulation_02, and simulation_03). Consequently, the increase of IMC thickness becomes slower and the depletion of Al layer takes longer time which is up to 100 hours in simulation_02. However, the total IMC thickness reaches stagnation and exhibits a noticeably higher value than measured from experiments. The reduced diffusivity data of Au rich phases is additionally applied in simulation_03. It is found that the simulated IMC growth shows quite converged tendency as observed from the experiments. The increase of total IMC thickness and the depletion of Al layer agree with experiment results well. This demonstrates that IMC diffusion simulation can be reasonably performed if the provided diffusivity data are accurate.

Since the IMC formation simulation presented above is based on the diffusion controlled assumption, chemical reaction is not considered in the simulation model. Therefore, if chemical reaction is the dominant mechanism during IMC formation, it cannot be simulated by the present methodology. Besides that, it is assumed in the simulation that atomic concentration is always continuous, which is actually not the case for IMC formation process [7]. Usually there is a discontinuity at phase boundaries and multiple stoichiometric phases are formed in such multi-component systems [14-16]. Nevertheless, the discussed simulation approach in this

study is fairly cost saving in time. For a fast estimation and prediction of IMC growth, it is of great benefit for industrial applications.

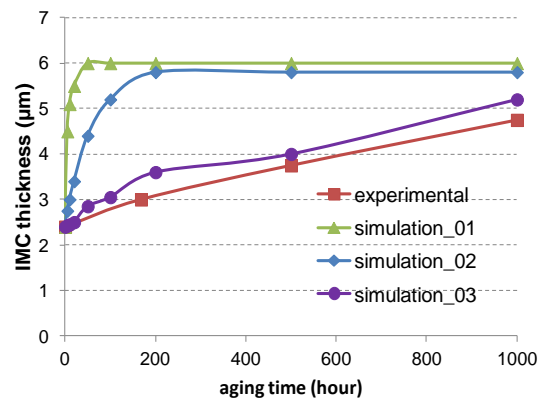


Figure 4: The development of total IMC thickness is shown as function of thermal aging time. Parametric study from simulation is in comparison with experimental results.

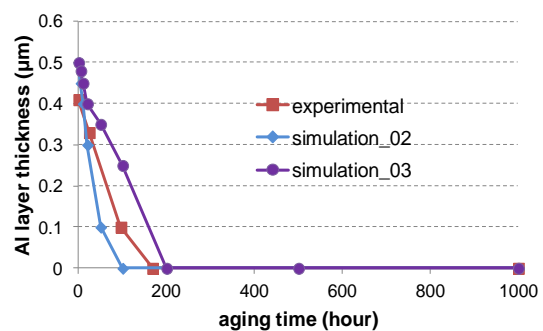


Figure 5: The depletion of Al layer is shown as function of thermal aging time. Parametric study from simulation is in comparison with experimental results.

3. The Concept of Subsequent Stress Analysis during IMC Formation

Only knowing the diffusion profile or overall IMC thickness is not sufficient for industrial application. In order to target the critical locations or phases in Au/Al wire bonds, it is necessary to further study subsequent stress analysis during IMC formation. The ultimate goal of the diffusion simulation is to investigate the stress evolution and distribution during IMCs formation. The similarity between diffusion simulation and thermal simulation provides a guide and pave a path to discover the feasibility of stress analysis. In a thermo-mechanical simulation, stress analysis can be performed, in which thermal stress is induced either by temperature gradients or thermal expansion mismatch. Consequently, stress σ can be calculated based on a temperature distribution profile and coefficient of thermal expansion α_T as below:

$$\sigma = \frac{E\alpha_T}{1-\nu}(T_1 - T_2) \quad (7)$$

where E is the elastic modulus, ν is the Poisson's ratio, and T_1, T_2 are temperatures at two states.

For intermetallic growth, on the one hand, it is a common belief that during the growth of compounds, the interfacial stresses and stress gradients serves as additional driving force to accelerate diffusion. On the other hand, due to different specific volumes of newly formed phases, stresses can be induced due to volume change. The later one is similar to the case described above for thermal induced stresses. Therefore, in order to perform an atomic diffusion induced stress analysis, it requires two key variables: the atomic concentration C and its related coefficient of volume change α_v , which can be expressed by the equation below:

$$\alpha_v = \frac{1}{3V} \frac{dV}{dC} \quad (8)$$

where V represents the atomic volume. Afterwards, stress induced by IMCs mismatch can be also calculated with equation (9) which is similar to equation (7).

$$\sigma = \frac{E\alpha_v}{1-\nu} (C_1 - C_2) \quad (9)$$

The profile of atomic concentration can be obtained directly from IMCs diffusion simulation as described in section 2. The difficult part is to derive a model which associates the volume change with the atomic concentration in order to acquire the coefficient of volume change α_v quantitatively.

The first possible way to model volume change with respect to atomic concentration is to use the atomic packing factor (APF) defined as the fraction of volume in a crystal structure which is occupied by atoms (Equation (10)).

$$APF = \frac{\sum N_{atoms} V_{atoms}}{V_{unit.cell}} \quad (10)$$

where N_{atoms} is the number of atoms in the unit cell, V_{atoms} is the volume of an atom, and $V_{unit.cell}$ is the volume occupied by the unit cell. The calculated APF values for Cu/Al and Au/Al compounds are summarized in Table 3 [3, 6].

Table 3: APF of Al, Cu, Au and intermetallics formed at interfaces.

Phase	APF	Phase	APF
Cu	0.74	Au	0.74
Cu ₉ Al ₄	0.776	Au ₄ Al	0.25
CuAl ₂	0.739	Au ₈ Al ₃	0.72
Al	0.74	Al	0.74

APF is dimensionless and always less than unity. The higher APF value represents the higher packing density, and accordingly the less volume. Al, Au and Cu are all face centered cubic (FCC) metals with the highest packing density. Because the APF of CuAl₂ is very close to that of pure metals and the APF of Cu₉Al₄ is 5% higher than that of CuAl₂ and other pure metals, IMC formation results in the loss of total IMC volume which leads to the increase of free volume for the possible void formation. The observed void formation at the Cu₉Al₄/Cu and Cu₉Al₄/CuAl₂ interfaces from experiments is thus interpretable [2, 3, 7, 9, 10, 18]. Unfortunately, transformation of the pure metals to Au/Al intermetallics

with lower APF results in an increase in IMC volume which is completely contradicted to the case of Cu/Al. From the experiments [1, 5, 6, 11, 12], it is observed that void formation is more likely to appear in Au₄Al phase. Hereby, this raises the question whether APF is the proper variable to model the volume change of IMC formation. Furthermore, it is also worthy to note that APF is a local microscopic variable. Compared to the volume change as a macroscopic variable, it is not straight forward to correlate APF with the volume change. Therefore, an intermediate model which can transform APF to volume change is required.

Another potential way to associate the volume change with atomic concentration is to use the molar volume. The molar volumes of the phases can be calculated using the following equation:

$$V_m = V_c N_a / Z \quad (11)$$

where V_m is the molar volume of phase, V_c is the volume of the unit cell, N_a is the avogadro constant $6.022 \times 10^{23} \text{ mol}^{-1}$, and z is the number of formula weights per unit cell. Xu [10, 12, 18, 19] has summarized the molar volume of all the possible phases in Au/Al and Cu/Al bonds as shown in Table 4.

Table 4: molar volume of Al, Cu, Au and intermetallics formed at interfaces.

Phase	Molar volume (cm ³ /mol)	Phase	Molar volume (cm ³ /mol)
Au	10.21	Cu	7.11
Au ₄ Al	49.95	Cu ₉ Al ₄	99.37
Au ₈ Al ₃	109.11	CuAl	16.90
Au ₂ Al	28.68	CuAl ₂	27.03
AuAl	20.36	Al	10.00
AuAl ₂	32.48		
Al	10.0		

Thus, volume changes due to IMC formation can be estimated as shown in Table 5 and 6, using the molar volumes listed in Table 4.

Table 5: Volume changes due to IMC formation at Cu/Al interface

Reactions	Volume change (%)
Cu+2Al->CuAl ₂	-0.30
9Cu+4Al->Cu ₉ Al ₄	-4.44
CuAl ₂ +Cu->2CuAl	-1.00
Cu+Al->CuAl	-1.23
4CuAl+5Cu->Cu ₉ Al ₄	-3.66
2CuAl ₂ +7Cu->Cu ₉ Al ₄	-4.30

Table 6: Volume changes due to IMC formation at Au/Al interface

Reactions	Volume change (%)
4Au+1Al->Au ₄ Al	-1.75
8Au+3Al->Au ₈ Al ₃	-2.30
2Au+Al->Au ₂ Al	-5.72
Au+Al->AuAl	0.74
Au+2Al->AuAl ₂	7.51
4Au+Au ₈ Al ₃ ->3Au ₄ Al	-0.07
2Au ₄ Al+Al->Au ₈ Al ₃	-0.72
2Au+Au ₂ Al->Au ₄ Al	1.73
3Au+AuAl->Au ₄ Al	-2.04

7Au+AuAl ₂ ->2Au ₄ Al	-3.90
Au+AuAl ₂ ->2AuAl	-4.61
3Au+AuAl ₂ ->2Au ₂ Al	-9.11
13Au+3AuAl ₂ ->2Au ₈ Al ₃	-5.19
Au+AuAl->Au ₂ Al	-6.18
5Au+3AuAl->Au ₈ Al ₃	-2.69
2Au+3Au ₂ Al->Au ₈ Al ₃	2.49

For the intermetallic growth and phase transformation of Cu/Al compounds, it always results in volumetric shrinkage. Most of compounds formed at Au/Al interface also have the volume reduction except for the formation of AuAl₂ which shows a significant increase 7.51% of the volume. It can be argued that AuAl₂ is a transitional phase and its subsequent transformations to AuAl and Au₂Al which have the 4.61% and 9.11% respectively can compensate the volume increase which also leads to the entire volume shrinkage at the end. Consequently, as stated by Xu [12] the stresses arising from the volume reduction can be relieved by the initiation and propagation of voids at weak regions. Similarly to that, Stephenson [20] and Paritskay and Bogdanov [21] proposed that void formation between different phases of IMCs can be attributed to the large plastic stresses which are induced by the IMCs phases due to their significant differences in volume.

Though molar volume is a more proper variable than APF to be used to calculate volume change during IMC formation, it still needs further development in order to be able to implement the coefficient of volume change α_v as one of material properties in a diffusion-mechanical coupled simulation. The modeling of the coefficient of volume change α_v in this study is still ongoing.

4. Conclusions

The paper develops and explores the use of a thermal analogue to model the intermetallic diffusion by commercial FEM software during wire bonding process. This allows the routine use of ANSYS to investigate the IMCs phase formation and thickness development, which can assist the understanding of intermetallic formation. Several scenarios with different parameter settings are simulated and good agreement is reached with the experimental observations. The discussions of the subsequent stress analysis due to the intermetallic formations are also presented.

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References

1] F. W. Wulff, C. D. Breach, D. Stephan, and K. J. Dittmer, "Characterisation of intermetallic growth in copper and gold ball bonds on

- aluminium metallization," EPTC, Ed.: IEEE, 2004, pp. 348-353.
- [2] M. Drozdov, G. Gur, Z. Atzmon, and W. Kaplan, "Detailed investigation of ultrasonic Al-Cu wire-bonds: I. Intermetallic formation in the as-bonded state," *Journal of Materials Science*, vol. 43, pp. 6029-6037, 2008.
- [3] M. Drozdov, G. Gur, Z. Atzmon, and W. Kaplan, "Detailed investigation of ultrasonic Al-Cu wire-bonds: II. Microstructural evolution during annealing," *Journal of Materials Science*, vol. 43, pp. 6038-6048, 2008.
- [4] H. J. Kim, J. Y. Lee, K. W. Paik, K. W. Koh, J. Won, S. Choe, J. Lee, J. T. Moon, and Y. J. Park, "Effects of Cu/Al intermetallic compound (IMC) on copper wire and aluminum pad bondability." vol. 26, I. T. o. C. a. P. Technologies, Ed., 2003.
- [5] C. Breach and F. Wulff, "Intermetallic growth in gold ball bonds aged at 175°C: comparison between two 4N wires of different chemistry," *Gold Bulletin*, vol. 42, pp. 92-105, 2009.
- [6] A. Karpel, G. Gur, Z. Atzmon, and W. Kaplan, "TEM microstructural analysis of As-Bonded Al-Au wire-bonds," *Journal of Materials Science*, vol. 42, pp. 2334-2346, 2007.
- [7] C. D. Breach and F. W. Wulff, "A brief review of selected aspects of the materials science of ball bonding," *Microelectronics Reliability*, vol. 50, pp. 1-20, 2011.
- [8] C. Ulrich, "Diffusion kinetics in aluminum-gold bond contacts from first-principles density functional calculations," *Acta Materialia*, vol. 59, pp. 7634-7644, 2011.
- [9] C. J. Hang, C. Q. Wang, M. Mayer, Y. H. Tian, Y. Zhou, and H. H. Wang, "Growth behavior of Cu/Al intermetallic compounds and cracks in copper ball bonds during isothermal aging," *Microelectronics Reliability*, vol. 48, pp. 416-424, 2008.
- [10] H. Xu, C. Liu, V. Silberschmidt, and Z. Chen, "Growth of Intermetallic Compounds in Thermosonic Copper Wire Bonding on Aluminum Metallization," *Journal of Electronic Materials*, vol. 39, pp. 124-131, 2009.
- [11] C. D. Breach and F. Wulff, "New observations on intermetallic compound formation in gold ball bonds: general growth patterns and identification of two forms of Au₄Al," *Microelectronics Reliability*, vol. 44, pp. 973-981, 2004.
- [12] H. Xu, "Thermosonic ball bonding: a study of bonding mechanism and interfacial evolution," Loughborough University, 2010.
- [13] J. Svoboda, I. Turek, and F. D. Fischer, "Application of the thermodynamic extremal principle to modeling of thermodynamic processes in material sciences," *Philosophical Magazine*, vol. 85, pp. 3699-3707, 2005.
- [14] J. Svoboda, F. D. Fischer, and R. Abart, "Modeling of diffusional phase transformation in

- multi-component systems with stoichiometric phases," *Acta Materialia*, vol. 58, pp. 2905-2911, 2010.
- [15] J. Svoboda, E. Gamsjäger, F. Fischer, and E. Kozeschnik, "Modeling of kinetics of diffusive phase transformation in binary systems with multiple stoichiometric phases," *Journal of Phase Equilibria and Diffusion*, vol. 27, pp. 622-628, 2006.
- [16] T. C. Illingworth and I. O. Golosnoy, "Numerical solutions of diffusion-controlled moving boundary problems which conserve solute," *Journal of Computational Physics*, vol. 209, pp. 207-225, 2005.
- [17] Y. Guo, G. Liu, H. Jin, Z. Shi, and G. Qiao, "Intermetallic phase formation in diffusion-bonded Cu/Al laminates," *Journal of Materials Science*, vol. 46, pp. 2467-2473, 2010.
- [18] H. Xu, C. Liu, V. V. Silberschmidt, S. S. Pramana, T. J. White, Z. Chen, and V. L. Acoff, "Behavior of aluminum oxide, intermetallics and voids in Cu-Al wire bonds," *Acta Materialia*, vol. 59, pp. 5661-5673, 2011.
- [19] H. Xu, C. Liu, V. V. Silberschmidt, S. S. Pramana, T. J. White, Z. Chen, M. Sivakumar, and V. L. Acoff, "A micromechanism study of thermosonic gold wire bonding on aluminum pad." vol. 108, *J. o. A. Physics*, Ed.: American Institute of Physics, 2010, p. 113517.
- [20] G. B. Stephenson, "Deformation during interdiffusion," *Acta Metallurgica*, vol. 36, pp. 2663-2683, 1988.
- [21] L. N. Paritskaya and V. V. Bogdanov, "Stress-Sensitive Effects in Diffusion Zone." vol. 129, *D. a. D. Forum*, Ed.: Trans Tech Publ, 1996, pp. 79-94.