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Interface Stresses Due to Imbalanced Diffusion in Wirebonding Between Gold (Au) and Aluminum (Al)

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ABSTRACT

Wirebonding is a fundamental process in semiconductor manufacturing, essential for creating reliable electrical connections between integrated circuits and their packaging. This paper explores the complexities of interface stresses arising from solid-state diffusion during wirebonding, with particular attention to the interactions between gold (Au) wires and aluminum (Al) bond pads. Due to the different diffusion rates of Au and Al atoms, intermetallic compounds (IMCs) form at the interface, playing a critical role in bond integrity. However, the growth of these IMCs also generates significant mechanical stresses, which can compromise the reliability and lifespan of wirebonded connections. Through detailed experimental analysis, this study investigates the kinetics of IMC growth, the influence of activation energy on diffusion, and the resulting microstructural evolution at bonded interfaces. By clarifying the mechanisms driving IMC formation and associated stresses, the paper offers insights into optimizing wirebonding processes. These include the selection of suitable bonding parameters and materials to reduce stress and enhance the performance and durability of semiconductor devices. Ultimately, the findings support the advancement of wirebonding techniques aimed at improving the reliability and efficiency of semiconductor packaging.

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1. INTRODUCTION

Wirebonding is a pivotal process in semiconductor manufacturing, serving as a key method for establishing electrical connections between integrated circuits (ICs) and their packaging. The process involves intricate physical and chemical interactions that directly influence the performance and reliability of electronic devices. One of the major challenges in wirebonding is interface stress, which develops during solid-state diffusion when thermal energy is applied to bond dissimilar materials such as gold (Au) wires and aluminum (Al) bond pads. These stresses primarily result from the unequal diffusion rates of the constituent atoms and the subsequent formation of intermetallic compounds (IMCs) at the interface. While IMCs are essential for ensuring strong and reliable bonds, their formation can also introduce localized stresses and potential failure sites within the device (Akbar *et al*., 2019; Mokhtari *et al*., 2014).

The formation and growth of intermetallic compounds (IMCs) at the bond wire-bond pad interface during wirebonding are critical factors influencing the reliability and performance of semiconductor devices. Atomic diffusion across the interface, driven by heat, results in the development of IMCs that exert both beneficial and detrimental effects on the wirebond connection (Lall *et al*., 2017; Subramanian *et al*., 2019; Rongen *et al*., 2019). For example, the rapid growth of IMCs can consume the aluminum layer, undermining bond integrity and potentially leading to premature device failure.

When heat is applied during wirebonding, atoms at the interface acquire sufficient energy to overcome potential barriers, allowing them to diffuse across the boundary. This process follows Fick's first law, which states that the flux of a substance (J) is proportional to the concentration gradient, meaning that atomic movement is driven by differences in concentration across a given area. As a result, atoms migrate from regions of high concentration to regions of low concentration. In wirebonding, aluminum atoms from the bond pad diffuse toward the gold wire, creating a concentration gradient. This differential diffusion is influenced by material properties such as atomic number, activation energy, and bonding energy (Mokhtari *et al*., 2014; Blish *et al*., 2007; Osenbach *et al*., 2013). Because aluminum atoms are smaller and more mobile than gold atoms, they diffuse more rapidly, leading to the formation of intermetallic compounds (IMCs) such as Au_4Al, Au_2Al, and $AuAl_2$ (Ulrich *et al*., 2011).

The kinetics of IMC growth (governed by factors such as temperature, bonding time, and material composition) play a crucial role in the development of interface stresses. The imbalance in solid-state diffusion rates between aluminum and gold generates substantial stresses at the interface, leading to microstructural deformations that compromise the mechanical and electrical integrity of the bonds (Osenbach *et al*., 2013; Gubbels *et al*., 2012).

Solid-state diffusion is a key driver in the formation of IMCs at wirebond interfaces, with a direct influence on their reliability and performance. The growth of IMCs is primarily controlled by the activation energy of diffusion, which dictates the rate of atomic movement across the interface (Attari *et al*., 2018; Mokhtari *et al*., 2014; Tea *et al*., 2017). Based on the Arrhenius equation, the diffusion coefficient is exponentially dependent on activation energy, indicating that even minor variations in activation energy can cause substantial changes in IMC growth rates.

The activation energy for IMC formation in common wirebonding systems, such as gold-aluminum, has been reported to range between 0.7 and 1.0 eV, depending on the specific phases formed. Interface stresses arising during IMC growth can be attributed to several mechanisms, including the Kirkendall effect, which promotes void formation and undermines bond integrity. Factors that influence activation energy and, consequently, IMC growth include material composition, surface conditions, and bonding parameters such as temperature and pressure (Lall *et al*., 2014; Liu *et al*., 2019; Attari *et al*., 2018).

The microstructural evolution of IMCs in wirebonding, driven by solid-state diffusion, is a critical factor influencing interface stress and overall bond integrity. During wirebonding, thermal energy promotes the diffusion of atoms between the bond wire, typically gold (Au), and the bond pad, usually aluminum (Al). This process leads to the formation of IMCs such as Au_4Al, Au_8Al_3, $AuAl_2$, and AuAl, whose microstructures evolve as functions of temperature and bonding conditions (Blish *et al*., 2007; Mokhtari *et al*., 2014; Osenbach *et al*., 2013).

Initially, a thin IMC layer forms at the interface. With continued diffusion, these IMCs grow and transform, altering their microstructure. The intrinsic properties of Au and Al strongly influence this process; the high diffusivity of Au and the strong affinity of Al for Au promote rapid IMC formation. The rate of IMC growth is highly dependent on factors such as temperature, bonding time, and the fundamental properties of the materials involved (Blish *et al*., 2007; Jiang *et al*., 2010).

Therefore, this study investigates the interface stresses induced by solid-state diffusion in wirebonding between gold (Au) wires and aluminum (Al) bond pads, with a focus on the formation and growth of intermetallic compounds (IMCs) and their impact on bond reliability. Specifically, it aims to analyze diffusion imbalances during wirebonding and their contribution to interface stress. By examining diffusion kinetics, activation energy, and the microstructural evolution of IMCs, this research seeks to generate insights for optimizing wirebonding processes to improve the performance and durability of semiconductor devices.

2. METHOD

The gold wires used in this experiment were fabricated from 99.999% (5N) purity gold ingots doped with calcium and beryllium, yielding 99.99% (4N) purity gold wire. The 4N gold wire exhibited a resistivity of 2.3 µΩ·cm, an elastic modulus of 75-100 GPa, and a tensile strength of 140–340 MPa. To achieve a high-strength, fine-grained structure, 1 % palladium was added to the 4N gold ingot, producing 2N gold wire. Palladium was selected due to its high solubility in gold and excellent corrosion resistance. The 2N gold wire showed a resistivity of 3.0-3.5 µΩ·cm, an elastic modulus of 80-95 GPa, and a tensile strength of 250-340 MPa. The copper wire was prepared from 99.999% (5N) copper using re-electrolysis and zone refining techniques.

All wires were drawn to a diameter of 25 µm through cold working, which introduced high internal stress and strain-hardening characteristics. To examine the relationship between microstructural and mechanical properties and bondability, the wires were annealed at temperatures ranging from 100°C to 600°C in 50°C increments for 10 seconds. Seven batches of each wire type (4N gold, 2N gold, and copper) were produced, and their surface hardness, tensile strength, and percentage elongation were measured. Optical microscopy and scanning electron microscopy (SEM) were employed to obtain cross-sectional images of the samples.

3. RESULTS AND DISCUSSION

3.1. IMC Growth Analysis

In this study, the effect of thin-film thickness on the rate of IMC growth was examined while maintaining a consistent grain size distribution. A nominal grain size of 700 nm was achieved through annealing heat treatment. Specifically, 4N gold wire was annealed at 500°C and subsequently bonded to substrates with five different thin-film thicknesses. During bonding, the parameters for each thickness were individually adjusted to ensure that all samples exhibited the same bond deformation ratio (b/h), where b denotes the bond width and h the bond height.

Figure 1 shows the IMC growth of 4N gold wire bonded onto substrates with varying thin-film thicknesses as a function of aging time. The results reveal that IMC thickness increases with aging time, characterized by an initial rapid growth phase followed by a stabilization period. After this initial stage, the growth rate decreases markedly and eventually stabilizes, suggesting a saturation point in the diffusion process.

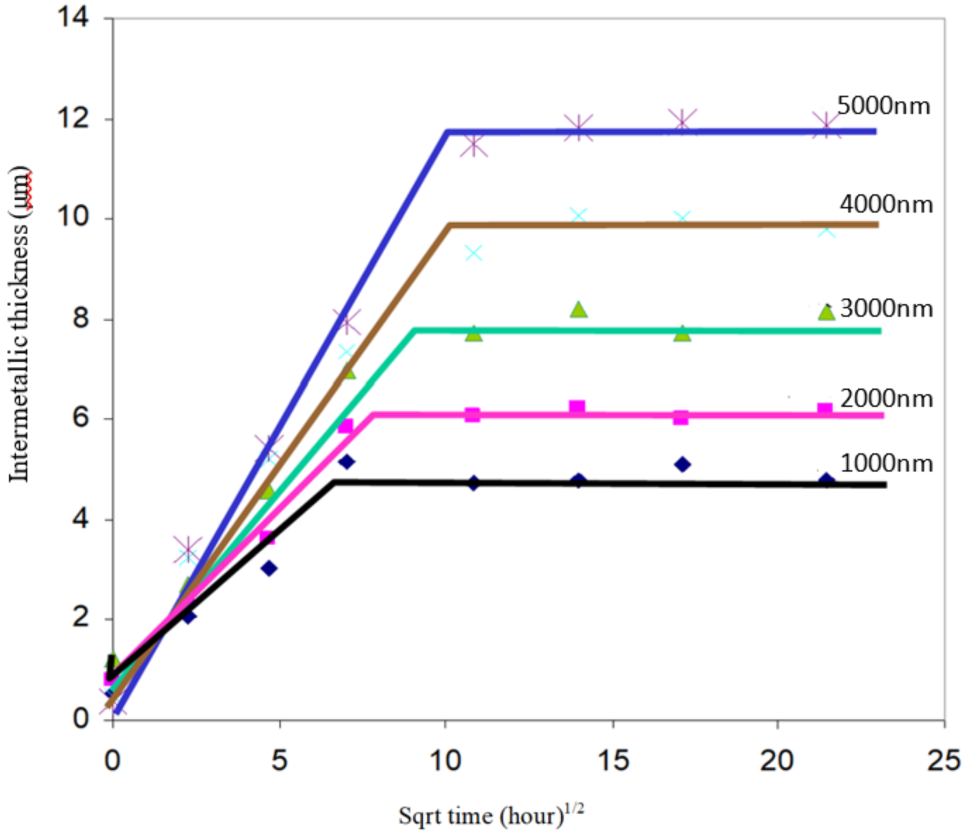

Figure 1. The intermetallic growth of 4N gold wire bonding on various thin film thicknesses as a function of aging time.

The rapid initial growth phase is attributed to the high concentration gradient between the gold wire and aluminum bond pad, which drives atomic diffusion. As the IMC layer develops, this gradient decreases, leading to a reduction in the diffusion rate. Such behavior is consistent with Fick's second law of diffusion, which predicts that the diffusion rate declines as the concentration gradient diminishes.

In the later stages of aging, the observed stabilization period indicates that the diffusion process approaches equilibrium, where the rate of IMC formation balances with atomic migration across the interface. This equilibrium is essential for the long-term reliability of wirebonded connections, as excessive IMC growth can increase brittleness and susceptibility to mechanical failure.

The uniform 700 nm grain size observed across all samples after annealing provides an essential basis for interpreting the diffusion kinetics. This structural consistency, regardless of the initial film thickness, indicates that the annealing process governs grain growth and establishes a stable microstructural environment for diffusion. Such uniformity allows the influence of film thickness on intermetallic growth to be more clearly isolated and accounts for the comparable initial growth rates across varying thicknesses. With grain sizes being consistent, the density of grain boundaries (commonly faster diffusion pathways than the bulk material) is likely similar in all samples. This supports the observation that the diffusion coefficient remains independent of film thickness, as illustrated in **Figure 2**.

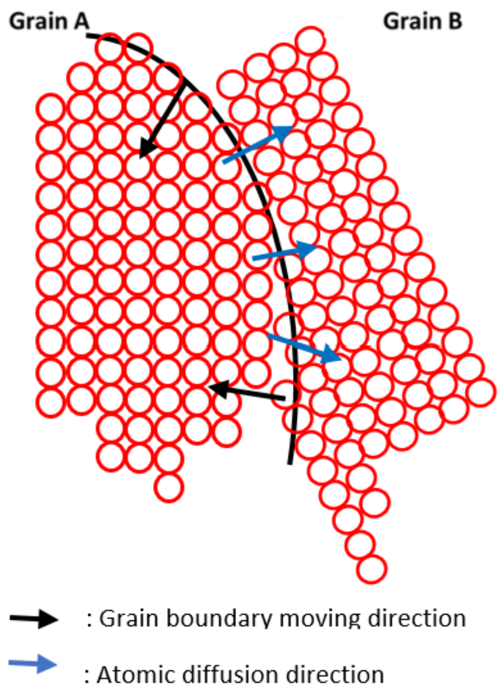

Figure 2. Atomic diffusion at a grain boundary occurs more easily compared to lattice diffusion due to the mismatch of atoms at the grain boundary.

The uniform microstructure across samples allows the differences in final intermetallic thickness to be attributed more directly to the amount of available material rather than to variations in diffusion pathways. It also adds weight to the observation of consistent time-to-plateau across thicknesses, suggesting that the depletion of thin-film material (rather than microstructural changes) is the primary factor governing the cessation of growth. This grain size consistency strengthens the reliability of the data by eliminating a potential source of variation between samples.

The results further demonstrate a clear correlation between thin-film thickness and IMC growth rate, with thicker films exhibiting faster growth. This trend underscores the importance of optimizing thin-film thickness to regulate IMC development and mitigate interface stress during the wirebonding process.

3.2. Activation Energy and Thin Film Thickness

The activation energy for intermetallic growth at various thin-film thicknesses was evaluated through thermal aging at 150, 200, and 250 °C (**Figure 3**). For 4N gold wire, thinner films (1000 nm) exhibited a lower activation energy of 0.46 eV, whereas thicker films (4000 nm) showed a higher activation energy of 0.72 eV. Comparing different wire materials, copper demonstrated the lowest activation energy, ranging from 0.29 to 0.64 eV, followed by 2N gold with values between 0.46 and 0.72 eV. In contrast, 4N gold wire showed the highest activation energy, ranging from 0.52 to 0.81 eV.

The variation in activation energy can be attributed to differences in the diffusion characteristics governing intermetallic compound formation, which play a critical role in determining the lifetime and overall reliability of wire bonds.

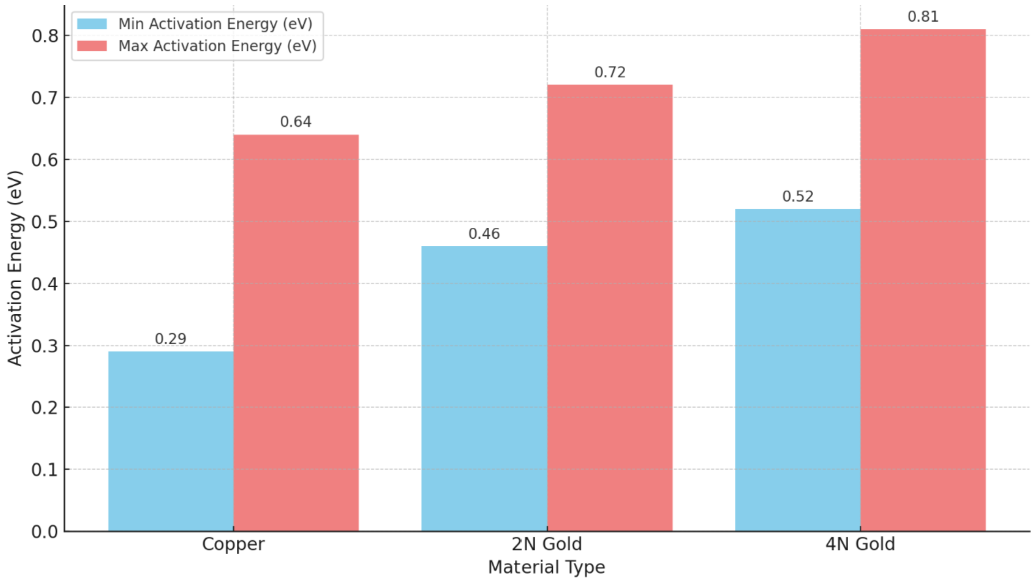

Figure 3. A bar chart comparing the activation energy versus the type of materials. The chart shows the minimum and maximum activation energy for copper, 2N gold, and 4N gold.

These findings are consistent with activation energy values reported in the literature, which typically range from 0.29 to 0.8 eV (Lee *et al*., 2018; Wang *et al*., 2020). The observed variation in activation energy can largely be attributed to differences in material type and their intrinsic properties (Mazloum-Nejadari *et al*., 2018).

Activation energy is a critical parameter in understanding diffusion phenomena, as it represents the minimum energy required for atoms to cross the interface and form intermetallic compounds. A lower activation energy indicates that less thermal energy is needed for atomic migration, thereby accelerating the formation and growth of intermetallic compounds. In contrast, a higher activation energy requires greater thermal input, leading to slower development of intermetallic compounds (Xu *et al*., 2007; Blish *et al*., 2007).

The reduced activation energy observed in thinner films can be attributed to their higher surface area-to-volume ratio, which enhances atomic mobility and accelerates diffusion processes as well as the formation of intermetallic compounds. In contrast, thicker films have a lower surface area-to-volume ratio, which restricts atomic mobility and thereby slows down diffusion phenomena, as shown in **Figure 4** (Wang *et al*., 2021; Wang *et al*., 2019). **Figures 4(a)** and **(b)** are the images for thin and thick films, respectively.

The variations in activation energy among different wire materials highlight the critical role of material selection in wire bonding processes. Copper's lower activation energy promotes the rapid formation of intermetallic compounds, which can be advantageous for applications requiring fast bonding and high productivity (Zhou *et al*., 2023). However, this accelerated IMC formation may also intensify interfacial stresses, raising potential reliability concerns. In contrast, gold's higher activation energy provides a more balanced diffusion rate, mitigating interfacial stress and making it a preferred choice for applications where long-term reliability and durability are essential (Quercia & Mancaleoni, 2016).

In conclusion, the analysis of activation energy provides valuable insights into the diffusion dynamics governing intermetallic compound formation in wirebonding (Zhou *et al*., 2023). The observed trend of lower activation energy in thinner films, along with the variations among different wire materials, highlights the necessity of deliberate material selection and process optimization to enhance bond reliability and ensure the long-term performance of wirebonded interconnections.

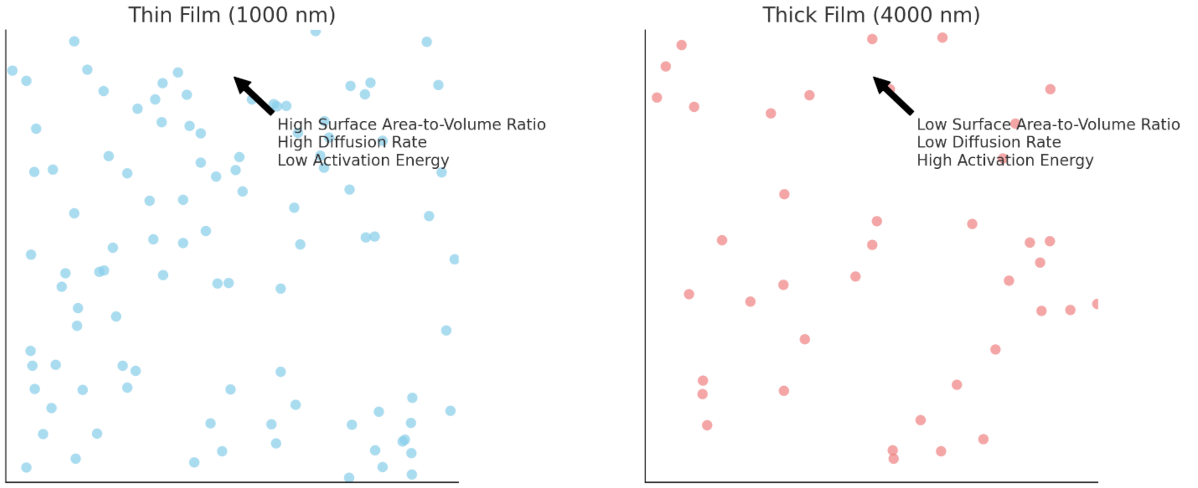

Figure 4. Comparison of the surface area-to-volume ratio between thin (a) and thick (b) films.

3.3. Microstructural Evolution and Mechanical Integrity

The microstructural evolution of intermetallic compounds (IMCs) during thermal aging plays a critical role in determining the mechanical integrity of wirebonded connections. As IMCs grow and transform, they undergo morphological and compositional changes that directly influence their mechanical behavior. The emergence of distinct IMC phases, such as Au_4Al, Au_8Al_3, $AuAl_2$, and AuAl, creates microstructural inhomogeneities at the interface, which in turn generate localized stress concentrations.

The coexistence of multiple IMC phases with differing mechanical properties generates regions of differential stress, where certain areas are subjected to higher tensile or compressive forces. These localized stresses can serve as initiation sites for crack formation and propagation, ultimately compromising the mechanical integrity of the bond. As IMCs evolve from a thin interfacial layer into a more complex and thicker microstructure, the severity of these stress concentrations intensifies, further amplifying the risk of mechanical degradation.

Experimental observations of wirebonded samples indicate that the growth and transformation of IMCs are frequently accompanied by the emergence of microstructural defects, including voids and cracks. These defects are predominantly associated with the Kirkendall effect, wherein the unequal diffusion rates of Au and Al generate vacancies at the interface. The accumulation of these vacancies promotes void formation, which can subsequently coalesce into cracks under mechanical loading or thermal cycling. **Figure 5** illustrates the influence of aging time on the development of intermetallic layer thickness for thin film thicknesses of 2000 and 4000 nm at different aging durations.

The analysis of wirebonded samples subjected to different aging durations reveals a clear correlation between IMC growth rate and the occurrence of microstructural defects. Samples exposed to longer aging times exhibit thicker IMC layers along with a higher density of defects, indicating that elevated temperatures combined with prolonged exposure accelerate diffusion and promote the formation of stress-inducing defects. In contrast, samples aged for shorter durations show slower IMC growth and fewer defects, suggesting that reduced exposure time mitigates diffusion and minimizes defect formation.

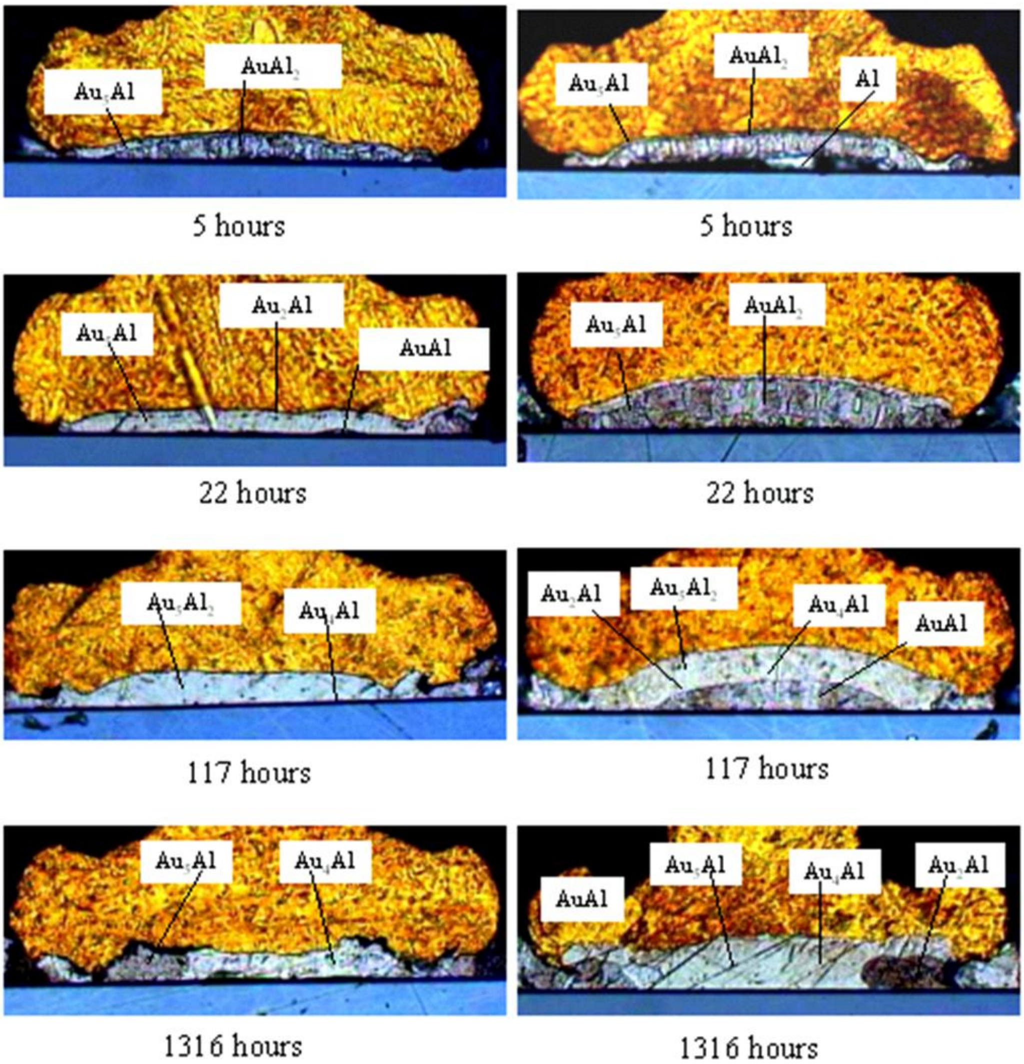

Figure 5. Influence of aging time on the development of intermetallic layer thickness for thin film thicknesses of 2000 and 4000 nm at different aging durations.

The influence of these microstructural changes on the mechanical integrity of wirebonded connections highlights the critical importance of optimizing thermal aging conditions. Careful control of both temperature and duration during thermal aging can effectively regulate the growth and transformation of IMCs, thereby minimizing the formation of stress-inducing defects and ultimately enhancing the long-term reliability of the bond.

4. CONCLUSION

This study examined the interface stresses induced by imbalanced diffusion in Au–Al wirebonding, with particular emphasis on the effects of thin film thickness, activation energy, and the microstructural evolution of intermetallic compounds (IMCs). The findings confirmed that the uniform grain size across samples enabled clear attribution of IMC growth variations to the availability of material rather than differences in diffusion pathways. IMC growth exhibited an initial rapid phase followed by a plateau, governed by the depletion of thin film material, underscoring the importance of diffusion kinetics in determining bond stability. Activation energy analysis demonstrated that thinner films facilitated faster IMC growth due to lower energy barriers, while thicker films exhibited higher activation energies and slower diffusion kinetics. Microstructural observations further revealed that prolonged aging promoted the formation of multiple IMC phases, as well as the development of voids and cracks through mechanisms such as the Kirkendall effect, ultimately compromising mechanical integrity.

Overall, the findings demonstrate that the diffusion imbalance between Au and Al is a primary source of interface stress, with thin film thickness and activation energy serving as key factors governing IMC growth and defect formation. By optimizing bonding parameters and carefully selecting materials, stress concentrations can be mitigated, voiding can be reduced, and the long-term reliability of wirebonded interconnections can be enhanced. This study provides a deeper understanding of diffusion-driven reliability challenges in semiconductor packaging and offers practical guidance for developing more robust and durable wirebonding processes.

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6. AUTHORS' NOTE

The author declares that there is no conflict of interest regarding the publication of this article. The author confirmed that the paper was free of plagiarism.

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