# PARAMETRIC DESIGN OF WIRE PASSIVATION THICKNESS TO REDUCE OXIDATION AND ELECTROMIGRATION RISKS IN MICROELECTRONIC PACKAGING

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## *ABSTRACT*

Reliability threats in advanced microelectronic packaging have increasingly emerged from coupled degradation mechanisms, focusing on oxidation and electromigration as miniature structures elevate current densities and thermal exposure. In this study experimental characterization of AuPCC wires and computational modeling are integrated to understand and identify the optimal passivation coating for Cu wires that would provide zero synergistic failure modes in AuPCC bonding on Au bond pad. Accelerated oxidation test using cyclic corrosion testing ASTM G85, Electromigration (EM) test ASTM F1996-00 and XPS testing showed 610nm-187nm as the passivation thickness range that could effectively suppress oxide breakthrough and minimizes EM-induced degradation

A coupled 2D numerical model, incorporating modified oxidation kinetics and drift-diffusion-based electromigration transport equations, was developed to replicate these experimental trends. Simulation results demonstrated 50 um bonding wires, requiring a minimum of 100nm passivation layers to significantly delay oxide penetration and inhibit galvanic formation. The suppression of early-stage diffusion and late-stage electric field-driven mass transport through the surface passivation applied coating enabled precise optimization of AuPd coating thickness to decouple oxidation and electromigration effects, thereby improving long-term wire reliability in next-generation microelectronic packages.

## 1. 0 INTRODUCTION

In semiconductor packaging, the transition to finer interconnect geometries and higher functional densities has amplified the significance of reliability concerns tied to metal line degradation. Two dominant phenomena, oxidation and electromigration can independently undermine interconnect performance, but when coupled, they often accelerate device failures more dramatically than either mechanism alone. As wire diameters shrink and current demands grow, surface oxidation weakens the protective barrier, promoting localized electron wind effects that exacerbate atomic diffusion, while EM-induced voiding exposes fresh metal to oxidation, forming a detrimental feedback loop.

Copper-based bonding wires, often employed with thin Au or Pd coatings are developed to enhance corrosion and oxidation resistance. In these instances, optimization of passivation layer thickness becomes critical, balancing costs against reliability improvements. Prior studies by Pan[1] et.al and Tu[2] et.al, explored either oxidation kinetics or EM lifetimes in isolation. However, comprehensive investigations that simultaneously model and validate the intertwined evolution of oxide growth and electromigration mass transport under operational conditions remain scarce.

This work addresses that gap by integrating laboratory characterizations with a tailored computational framework to predict how the passivation thickness of AuPd on Cu wires modulates the coupled oxidation and EM degradation pathways of the bonding wire. These insights allow packaging engineers and manufacturers to be informed beforehand of the reliability-centric parametric design of bonding wires surface passivation, aligning it with modern packaging requirements.

## 2.0 REVIEW OF RELATED WORK

### *2.1 Oxidation Dynamics in Copper-Based Interconnects*

Copper (Cu) interconnects, while widely used for their excellent electrical and thermal properties, are inherently vulnerable to oxidation especially in high-temperature and humid conditions typical of many packaging environments. The oxidation process follows a parabolic growth law, indicating that oxide thickness increases more slowly over time due to the diffusion-limited nature of the reaction. This can be described by the equation:

$$x^2 = k_p t \qquad \text{(Eq.1)}$$

where $x$ is the oxide layer thickness, $t$ is the exposure time, and $k_p$ is a rate constant influenced by temperature and oxygen partial pressure.

To reduce oxidation, a thin passivation layer of either a dopant or flash coating is often applied to the wire surface. This layer slows down oxygen ingress effectively. However, even well-deposited coatings can have weak points, such as grain boundary pathways or microdefects, where localized oxidation can initiate. Over time, this localized damage can compromise wire integrity, particularly under conditions involving repeated thermal cycling, which stresses interconnect reliability.

### *2.2 Electromigration-Driven Mass Transport in Wires*

Electromigration (EM) refers to the movement of metal atoms driven by the momentum of electrons flowing under high current densities. Over time, this mass transport can cause voids or hillocks to form within the wire, eventually leading to electrical failure through open or short circuits. The risk increases with higher operating temperatures and when the wire's internal structure lacks sufficient resistance to atomic diffusion.

Tzheng[3] et al. explored the influence of microstructure on EM behavior in copper wires and observed that larger, columnar grains grown during free air ball (FAB) and stitch regions significantly showed reduced EM formation. These grain structures acted like highways for current barriers to atom movement, reducing the chance of void formation.

Pan[1] et.al, on the other hand tested palladium coated copper wires under high current stress and observed that the Pd layer played a protective barrier. Through the reduction of the surface and grain boundary diffusion of copper atoms, it extended wire life by nearly 50% compared to bare Cu wires. Liang[4] et al. took a simulation-based approach, combining finite element models of current and temperature with atomic-level diffusion behavior. Their work highlighted that the stitch bond is particularly vulnerable to EM damage due to current crowding which often exceeds $10^6$ A/cm$^2$, a trend also observed in real-world failures. In another manuscript, Schlesinger [5] et al. evaluated Cu, Ag, and Au wires under accelerated EM conditions to validate the best bonding wire that would offer the best conductivity, it also showed the lowest EM resistance because of its faster grain boundary diffusion rate. Liang[6] et al., reported similar findings, reinforcing the idea of the factors to quickly look at in any industries search for the most appropriate bonding wire, conductivity, effect on efficiency and effect on package reliability.

### *2.3 Interplay Between Oxidation and Electromigration*

Although oxidation and electromigration are often studied separately, recent research suggests they are closely linked in advanced microelectronic packaging. Zhang[7] et al. and Kim[8] et al. both reported that surface oxidation can increase roughness, leading to uneven surface uniformity, and uneven electric fields that further promote EM-driven atomic migration. Conversely, when EM causes voids to form, it can expose fresh wire surfaces that are more susceptible to rapid oxidation.

This cyclical relationship becomes increasingly important as packages become more compact and thermally stressed. In today's dense interconnect layouts, where thermal gradients and current crowding are unavoidable, the interaction between EM and oxidation creates a reliability challenge that must be addressed during design and material selection. Understanding how these two failure modes influence each other is key to extending the lifetime of Cu-based interconnects in modern devices.

## 3.0 METHODOLOGY

This study employed a combination of electromigration, corrosion exposure, and adhesion strength testing to characterize the environmental and thermal degradation behaviors of 50 µm AuPdCu wires from two different suppliers. The methodology was guided by established standards ASTM F1996-00 for metal migration, ASTM G85 for cyclic corrosion testing and incorporated Cu surface adhesion and oxidation assessments relevant to microelectronic packaging environments.

### *3.1 Cyclic Corrosion Exposure*

To simulate oxidative degradation during storage or handling prior to encapsulation, a cyclic corrosion test was conducted using 5% solution of sodium chloride (NaCl) and sodium sulfate ($Na_2SO_4$). Equal lengths of 50 µm AuPdCu wires from two different suppliers were mounted on non-reactive substrates with partial exposure to both solution and ambient air.

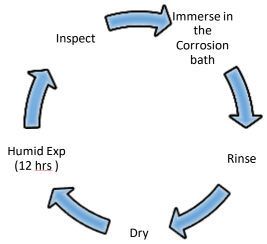

Fig. 1. Cyclic Corrosion Test

Samples were immersed in the corrosion solution for one hour, rinsed with deionized water, then thoroughly dried using an air blower. Following this, wires were allowed to rest in ambient air for 12 hours to simulate natural aging. This immersion-aging cycle was repeated to observe cumulative effects of corrosion and atmospheric exposure. Surface degradation and discoloration were evaluated using optical microscopy and high-resolution imaging, providing visual insight into corrosion susceptibility among the wire types.

### 3.2 Electromigration Testing

Electromigration behavior was evaluated following the guidelines of ASTM F1996-00 to simulate moisture-induced electromigration under voltage bias. Wires were cut to 6 cm lengths and mounted in parallel on a clean glass slide with a spacing of approximately 0.6–0.8 mm. A drop of distilled water was dispensed between the wire pair using a precision fluid micro dispenser. A pulsing DC voltage of either 5 V or 10 V was then applied across the wires for 5 minutes while the water droplet remained in contact as shown in Fig 2.

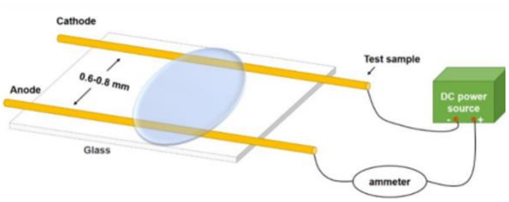

Fig 2. Schematic diagram of the electromigration test set-up.

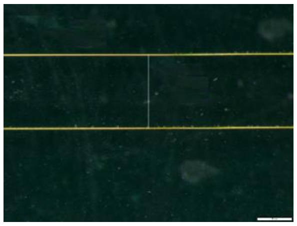

Fig. 3. Actual image of the wires set in a glass slide.

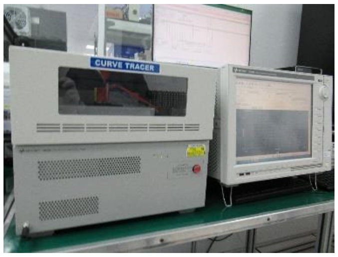

Fig 4. Actual image of the ammeter and the voltage source represented by an in-house curve tracer.

After bias exposure, the scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX) were used to assess dendritic growth and elemental migration. This procedure was repeated on plasma-cleaned wires from both suppliers to determine how surface treatment influences resistance to electromigration under humid, electrically stressed conditions.

### 3.3 Oxidation and Adhesion Strength Characterization

The oxidation behavior of copper surfaces and its impact on adhesion were characterized through X-ray Photoelectron Spectroscopy (XPS) and an in-situ oxide etching procedure. These tests were designed to evaluate the nature, thickness, and removability of copper oxides formed under thermal exposure. This also correlates surface chemistry with the risk of adhesion loss in downstream processes such as molding.
Wires were thermally aged at temperatures above 200 °C in both air and nitrogen environments to simulate conditions encountered during pre-mold and wire bonding processes. After exposure, XPS analysis was performed to determine the surface oxidation state. Spectral deconvolution focused on identifying the relative abundance of metallic copper ($Cu^0$), cuprous oxide ($Cu_2O$, $Cu^+$), and cupric oxide ($CuO$, $Cu^{2+}$). These oxidation states were used to infer the level of surface degradation and potential adhesion risk.
To further evaluate oxide removability, the thermally exposed samples were subjected to a mild wet etching process using a dilute acid-based solution. Etch response was monitored visually and confirmed through post-etch XPS to assess oxide layer persistence.

### 3.4 Cu Oxidation and Electromigration Modeling via Coupled Numerical Simulation

To deepen the understanding of reliability degradation mechanisms observed in wire bonds, a two-dimensional numerical model was developed which simulates the simultaneous effects of copper oxidation and electromigration. This integrated approach allowed for the prediction of oxide growth behavior and atom migration over time under realistic thermal and electrical stress conditions.

The thermal oxidation component of the model was governed by a modified Deal-Grove framework, which accounts for both the linear and parabolic regimes of oxide growth:

$$x^2 + Ax = B(t + \tau) \qquad \text{(Eq.2)}$$

Here, x is the oxide thickness, t is the exposure time, and $\tau\backslash\tau$ is a time offset representing initial oxide formation. The constants A and B represent linear and parabolic rate components, respectively, and are both temperature-dependent, expressed through Arrhenius relationships:

$$A(T) = A_0 \exp\left(-\frac{E_a^A}{kT}\right), \quad B(T) = B_0 \exp\left(-\frac{E_a^B}{kT}\right) \qquad \text{(Eq.3)}$$

Where $A_0$ and $B_0$ are pre-exponential factors, $E_a{}^A$ and $E_b{}^B$ are the activation energies, k is Boltzmann's constant, and T is the absolute temperature.

In parallel, the model incorporated a drift-diffusion formulation to describe electromigration-driven atomic transport:

$$J = -D\nabla C + \frac{Z^{*}eDC}{kT}\nabla\phi \qquad \text{(Eq.4)}$$

In this equation, J is the atomic flux, D is the diffusion coefficient, C is atomic concentration, $Z^{*}$ is the effective charge number, e is the elementary charge, and $\phi$ is the electrical potential. The first term represents concentration-gradient-driven diffusion, while the second captures the drift under an electric field, a key driver of mass transport in energized metal lines.

## 4.0 RESULTS AND DISCUSSION

### *4.1 Cyclic Corrosion Exposure*

Two set of wires from supplier A and supplier B are subjected to cyclic corrosion exposure. After just 1 hour of bath immersion, pitting corrosion was already evident on both types of wire. However, supplier B's wire exhibited fewer pits, indicating superior resistance to the corrosive elements present in the bath. Subsequent staging for 12 hrs inside the fume hood under ambient conditions (non-nitrogen environment) further revealed the progression of galvanic corrosion on both wire types, with visible propagation along the exposed surfaces.

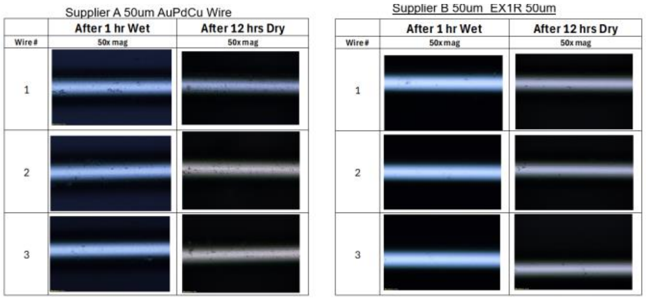

Fig 5. Cycle 1.Actual image of the evaluated wire samples after 1 hr of wet corrosion exposure and on the right, after 12 hrs of drying.

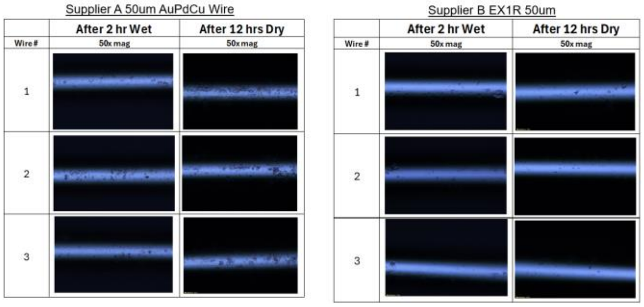

Fig 6. Cycle 2. Actual image of the evaluated wire samples after 2 hrs of wet corrosion exposure and on the right, after 12 hrs of drying.

After 2 hours of salt solution exposure, Supplier A wires exhibited excessive pitting, indicating severe material degradation. This degradation further intensified after 12 hours of ambient staging, with corrosion visibly progressing across the wire surface. In contrast, supplier B wires demonstrated significantly better performance, maintaining structural integrity and showing minimal corrosion even after the same 2-hour immersion period.

### *4.2 Electromigration Testing*

Under electromigration testing with a 5 V pulsed bias for 5 minutes, Supplier B's EX1R wire exhibited a more resistant surface, with only minimal formation of nodules and galvanic cells. In contrast, Supplier A's Au-flash Pd-coated wire showed more pronounced surface degradation, indicating greater susceptibility to electromigration-induced damage.

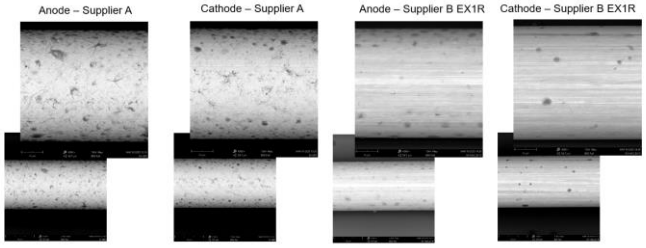

Fig 7. Electromigration Test results comparing Supplier A and Supplier B after 5V pulsed bias for 5 mins.

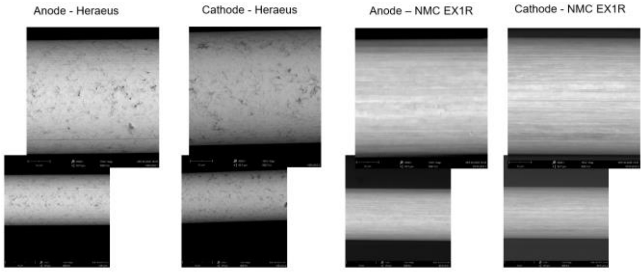

Fig 8. Electromigration Test results comparing Supplier A and Supplier B after 5V pulsed bias for 5 mins on wires subjected with ArH2 plasma prior EM test.

With $ArH_2$ batch plasma treatment applied to the wires prior to electromigration testing, a notable reduction in galvanic cell formation and oxidation nodule growth was observed across both wire types. Following a 5 V pulsed bias for 5 minutes, Supplier B's wires exhibited superior stability, with no visible signs of galvanic corrosion or oxidation nodules. In comparison, Supplier A's wires showed minor surface activity, indicating relatively higher susceptibility despite the plasma pretreatment. These results highlight the enhanced electromigration resistance of Supplier B's EX1R wire under accelerated stress conditions.

### *4.3 Oxidation and Adhesion Strength Characterization*

To understand how thermal exposure affects the surface integrity and adhesion reliability of AuPCC bonding wires, a series of controlled oven aging experiments were conducted. In the unaged (bare) condition, the wires exhibited a thin organic film on the surface, likely originating from anti-tarnish protection or handling residues. This layer remained relatively stable at lower temperatures.

| **Condition** | **Oven Type** | **Visual Observation** | **Oxide Composition** | **Oxide Layer Thickness & Remarks** |
|---|---|---|---|---|
| Bare | None | Thin organic layer | Possible anti-tarnish coating or handling residue | No significant oxidation; stable surface |
| 150 °C, 210 min | Box, Air | Dark brown color | Organic layer + $Cu_2O$ | 2nd layer: 40 nm $Cu_2O$; acceptable oxide type |
| 200 °C, 15 min | Box, Air | Dark blue to purple | Organic layer + CuO / $Cu_2O$ | 2nd layer: 40 nm $Cu_2O$, CuO forming; risk due to CuO onset |
| 200 °C, 30 min | Box, Air | Dark green | Organic layer + CuO | 2nd layer: 55 nm $Cu_2O$; increased risk from CuO development |
| 200 °C, 120 min | Box, Air | Green / silver-green | Organic layer + CuO / $Cu_2O$ | 2nd layer: 15 nm CuO; 3rd layer: 80 nm $Cu_2O$; distinct oxide layering |
| 200 °C, 150 min | Box, Air | Green / silver-green | Organic layer + CuO / $Cu_2O$ | 2nd layer: 10 nm CuO; 3rd layer: 170 nm $Cu_2O$; thick oxide, adhesion risk |

Table 1. Summary of Oxidation Characteristics of Cu Wires Under Oven Aging Conditions

### *4.4 Cu Oxidation and Electromigration Modeling via Coupled Numerical Simulation*

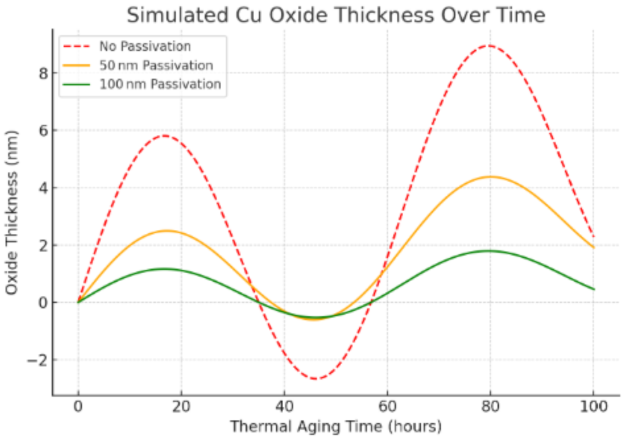

Fig 9. Simulated Cu Oxide thickness with thermal ageing of 100hours.

Fig 9, shows the simulated copper oxide growth over time, reflecting how different passivation thicknesses (0, 50 nm, 100 nm) impact the rate of oxidation. These trends align with the XPS observations where air-aged samples exhibited more persistent $Cu^{2+}$ species, indicating thicker oxide layers in the absence of passivation.

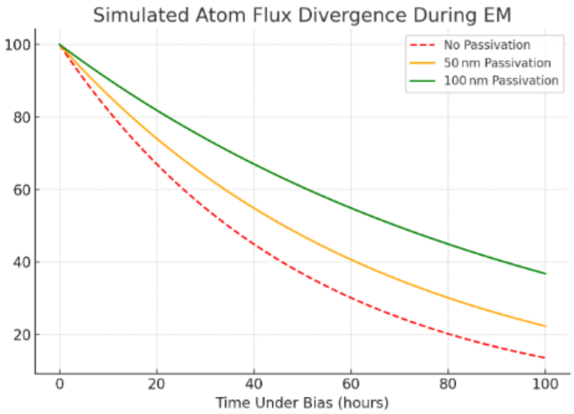

Fig 10. Simulated atomic flux divergence during electromigration for 100 hrs. under biased conditions.

Fig 10 illustrates the simulated atomic flux due to electromigration with 5V biased on wires with no passivation, 50nm passivation and 100 nm passivation. A thicker passivation layer significantly suppresses the divergence, corresponding with improved interfacial stability and reduced void formation risk, as indirectly supported by adhesion degradation trends in XPS study of section 4.3.

## 5.0 CONCLUSIONS

This study demonstrated the critical role of passivation thickness and surface pretreatment in improving wire bond reliability by mitigating oxidation and electromigration in microelectronic packaging. Experimental corrosion and electromigration tests revealed that Supplier B's EX1R wire consistently outperformed Supplier A's Au-flash Pd-coated wire, showing superior resistance to pitting and surface degradation under both environmental and electrical stress conditions.

Importantly, subjecting both wire types to $ArH_2$ batch plasma treatment prior to wire bonding resulted in a significant reduction in galvanic cell formation and oxidation nodule growth during electromigration testing. This surface conditioning step improved surface cleanliness and enhanced the stability of the wire under bias stress, particularly for Supplier B's wire, which exhibited no visible corrosion features post-testing.

Thermal aging experiments confirmed that unpassivated Cu wires rapidly develop complex oxide layers primarily $Cu_2O$ and CuO, that compromise adhesion integrity over time. Coupled numerical simulations supported these findings, showing that increasing passivation thickness (up to 100 nm) significantly suppresses oxidation growth and reduces atomic flux divergence during electromigration. These modeling results align with XPS-based compositional analysis, confirming the correlation between oxide evolution and interfacial degradation.

Collectively, these findings underscore the importance of integrating optimal passivation thickness and pre-bond plasma surface treatment as key design and process strategies to prolong wire bond reliability and ensure robust performance in advanced electronic packaging environments.

## 6.0 RECOMMENDATIONS

To enhance wire bond reliability and minimize the risks of oxidation and electromigration in microelectronic packaging, the following process and design improvements are recommended:

Adopt Wires with Proven Corrosion and EM Resistance: Selection of bonding wires with robust metallurgical stability—such as Supplier B's EX1R wire—should be prioritized due to their demonstrated resistance to pitting corrosion and electromigration-induced degradation under accelerated stress conditions.

Implement Optimized Passivation Thickness: A passivation layer thickness of at least 100 nm is recommended based on simulation and experimental correlation, as it significantly retards copper oxide growth and suppresses atomic flux divergence during electromigration, thereby enhancing interfacial integrity.

Integrate $ArH_2$ Plasma Treatment Prior to Wire Bonding: Pre-treatment of bonding wires using $ArH_2$ plasma is strongly advised to improve surface cleanliness, reduce initial oxide contamination, and enhance adhesion strength. This step is especially beneficial for minimizing galvanic cell formation during high-current or high-temperature exposure.

Limit Thermal Exposure During Assembly: Wire bond processing temperatures should be carefully controlled, ideally below 150 °C, to avoid rapid formation of detrimental oxide layers ($Cu_2O$/CuO) that compromise bond strength over time.

Continue Simulation-Aided Parametric Optimization: Further development and application of coupled multiphysics simulation models is encouraged for predictive design of wire materials and surface treatments under evolving packaging architectures and reliability expectations.

By implementing these recommendations, manufacturers can significantly improve the long-term performance and reliability of fine-pitch Cu wire bonding in advanced semiconductor packages.

## 7.0 ACKNOWLEDGMENT

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