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Predictive Reliability Modeling of Hybrid Bonding Through Warpage and Interfacial Defect Correlation

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***Abstract*—Hybrid bonding has become a cornerstone technology for enabling ultra-fine-pitch, high-density three-dimensional (3D) integration in advanced semiconductor packaging, including chip-on-wafer-on-substrate architectures. As interconnect dimensions continue to scale, bonding quality has grown increasingly sensitive to wafer-level non-uniformities and interfacial imperfections. In particular, pre-bond wafer warpage, bonding misalignment, and interfacial defects, including voids, delamination, and incomplete Cu–Cu or dielectric bonding, pose significant challenges to yield, reliability, and long-term device performance. In addition, A comprehensive taxonomy of hybrid-bonding defect modes across Cu–Cu, dielectric, and heterogeneous interface types is developed to enable systematic classification, correlation, and failure-mechanism identification. This work introduces a predictive reliability modeling framework that quantitatively links pre-bond warpage characteristics to post-bond interfacial defect formation. The proposed methodology integrates full-field warpage measurement using shadow moiré interferometry with high-resolution defect inspection through optimized scanning electron microscopy (SEM). The proposed framework facilitates data driven yield prediction, early-stage defect identification, and enhanced process control by linking deformation induced bonding variability with failure mechanisms. This approach addresses critical limitations in conventional inspection workflows and provides a scalable pathway toward predictive reliability modeling in advanced three-dimensional integration systems.**

***Index Terms*—Hybrid Bonding Reliability, Warpage Induced Defects, Shadow Moiré Interferometry, Yield Prediction**

I. Introduction

The increasing demand for high-performance computing, artificial intelligence, and data-intensive applications has accelerated the transition toward advanced semiconductor packaging paradigms that emphasize heterogeneous integration and three-dimensional architecture, as illustrated in Fig. 1 [1]. Hybrid bonding has emerged as a key enabling technology in this evolution, allowing for ultra fine pitch interconnects, reduced parasitic effects, and improved electrical and thermal performance compared to traditional packaging approaches. Architectures such as wafer-to-wafer and die-to-wafer bonding, as well as chip-on-wafer-on-substrate integration, rely heavily on the precision and reliability of hybrid bonding processes to achieve high interconnect density and functional integration [2].

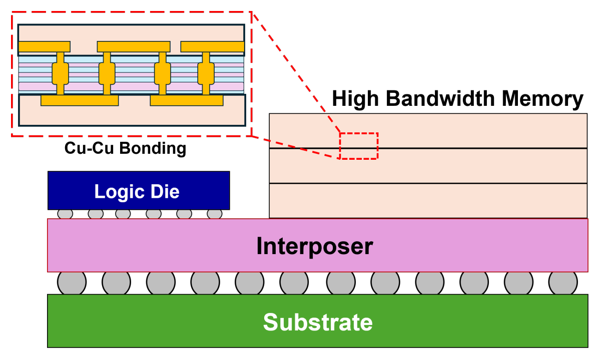

Fig. 1: Schematic of a three dimensional advanced packaging structure with Cu-Cu bonding

Despite these advantages, the continued scaling of bonding dimensions into the sub-micron regime has introduced new reliability challenges that are not adequately addressed by existing inspection and metrology techniques. At these scales, the tolerance window for bonding alignment and surface planarity becomes extremely narrow, making the process highly sensitive to even minor variations in wafer topography and material properties. Among the various factors influencing bonding quality, wafer warpage has emerged as one of the most critical parameters governing interfacial integrity.

Wafer warpage originates from multiple sources as mentioned in Fig. 2, including coefficient of thermal expansion mismatch between dissimilar materials, residual stresses introduced during thin film deposition, and structural asymmetry in multilayer stacks. In advanced packaging systems that integrate silicon, dielectric layers, and metallic interconnects, these effects are further amplified due to heterogeneous material interactions. Even small out of plane deviations on the order of micrometers can result in non-uniform contact during bonding, leading to localized gaps, incomplete metal to metal contact, and misalignment of bonding vias. These defects not only degrade electrical connectivity but also act as initiation

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sites for delamination and crack propagation under thermal or mechanical loading conditions.

A critical challenge in addressing these reliability issues lies in the limitations of existing inspection methodologies. Conventional pre bond metrology techniques, such as stylus profilometry and localized optical measurements, provide only point based information and are insufficient for capturing full field deformation behavior across the wafer. While these methods can verify local alignment or surface roughness, they fail to account for global curvature and spatial non uniformity, which are key contributors to bonding variability. As a result, wafers that satisfy pre bond inspection criteria may still exhibit hidden warpage induced defects that manifest after bonding, leading to yield loss and increased manufacturing cost.

On the other hand, post bond characterization techniques, particularly scanning electron microscopy, offer high resolution visualization of interfacial features but are inherently reactive in nature. These techniques are typically used to diagnose failures after they occur, rather than predict them. Furthermore, sample preparation processes such as focused ion beam sectioning introduce additional complexities, including redeposition, surface damage, and charging artifacts, which can obscure the true morphology of interfacial defects. This disconnects between pre bond inspection and post bond failure analysis represents a significant gap in current reliability assessment frameworks.

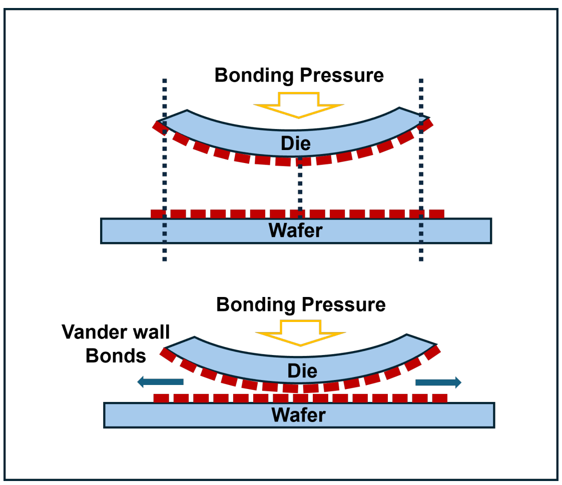

Fig. 2: Warped Die-Wafer bonding process showing a smiley thin die wafer bonding with a flat wafer by the initial vander wall bonding forces

To address these challenges, there is a growing need for integrated methodologies that can establish direct correlations between pre bond conditions and post bond outcomes. Such approaches would enable predictive reliability modeling, where potential failure mechanisms can be identified and mitigated prior to bonding. In this context, full field warpage characterization techniques, such as shadow moiré interferometry, provide a promising solution by enabling rapid, noncontact measurement of wafer deformation with high spatial resolution. When combined with optimized post bond defect characterization, these techniques can provide a comprehensive understanding of the relationship between deformation induced variability and interfacial defect formation.

In this work, a predictive reliability modeling framework is proposed that integrates pre bond warpage mapping with post bond interfacial defect analysis to establish a data driven correlation between deformation characteristics and failure mechanisms. A detailed taxonomy of hybrid bonding defects is developed to enable systematic classification across different interface types, including Cu Cu, dielectric, and heterogeneous material interfaces. By extracting key features from warpage profiles and defect distributions, the proposed framework facilitates the development of predictive models for defect probability and yield estimation [3].

The significance of this work lies in its ability to transition failure analysis from a reactive diagnostic approach to a predictive and data driven paradigm. By bridging the gap between inspection and reliability assessment, the proposed methodology provides a pathway toward improved process control, enhanced yield, and robust performance in advanced three-dimensional integration systems. Furthermore, the framework lays the foundation for the development of standardized defect signature libraries and machine learning driven reliability prediction tools, which are expected to play a critical role in the future of semiconductor manufacturing and packaging.

II. Taxonomy of Hybrid Bonding Defects

Hybrid bonding clearly involves interactions among many materials, including Copper (Cu), dielectric, and barrier materials; there isn't a clearly defined, categorized set of defects to understand them. To address this gap, we propose a detailed taxonomy of defects as illustrated in Fig. 3 across six interfaces in bonded W2W (Wafer to Wafer) or D2W (Die to Wafer) hybrid bonds. The interfaces are Cu-Cu, Dielectric-Dielectric, Barrier, Dielectric-Barrier, Cu-Barrier, Cu-Dielectric. Across these 6 interfaces, defects that affect interconnect functionality originate during fabrication. It is important to understand defects at the interfacial level to avoid recurring fabrication issues that cause them. Organizing defects by the six critical interfaces provides a physics-based framework for root-cause analysis, metrology selection, process optimization, and reliability modeling. Each interface governs a distinct aspect of interconnect performance: electrical resistance and electromigration (Cu-Cu), hermetic sealing and mechanical stiffness (Dielectric–Dielectric), diffusion blocking (Barrier-related interfaces), and interfacial adhesion and chemical stability (mixed-material interfaces).

A. *Cu-Cu Interface*

At the Cu–Cu interface, defects such as delamination, missed Cu contact, voids, Cu_2O formation, misalignment, edge delamination, bonding gaps, and missing pads directly compromise electrical conduction. Delamination at the Cu–Cu interface interrupts metallurgical continuity, increasing contact resistance and creating current-crowding sites that accelerate

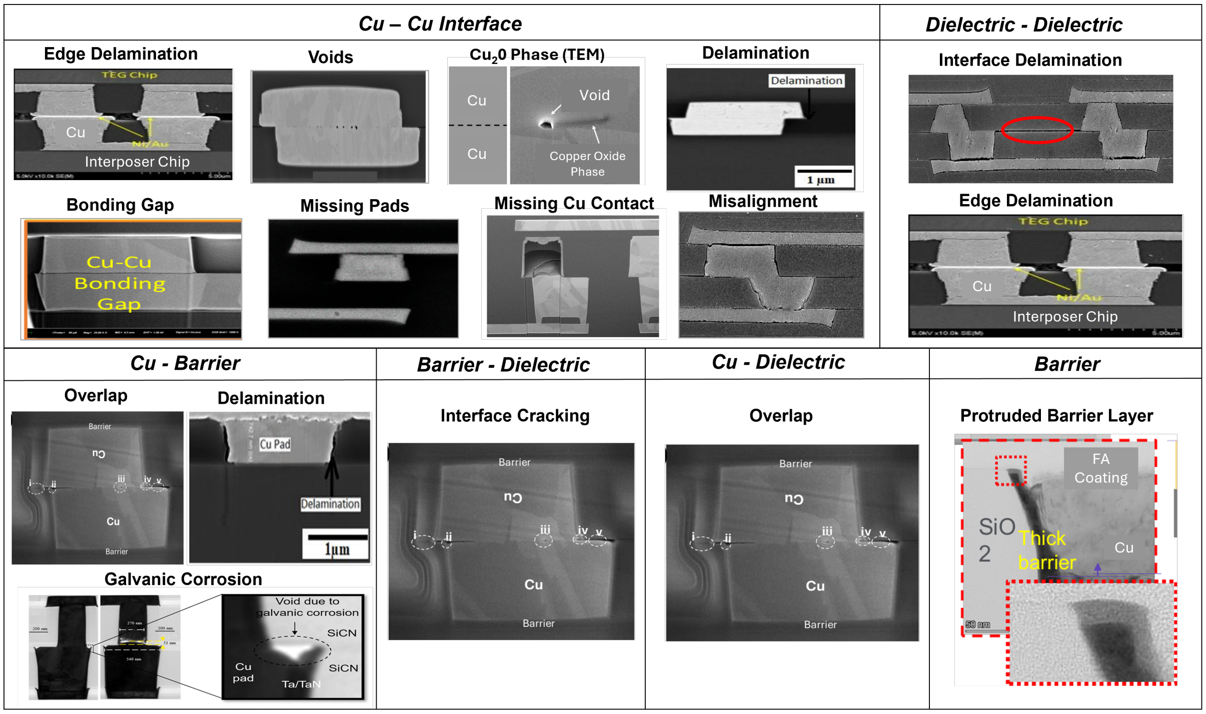

Fig. 3: A comprehensive hybrid bonding interfacial defect taxonomy [4-11]

electromigration. Missed Cu contacts and bonding gaps indicate incomplete interfacial bonding, effectively reducing the conductive cross-sectional area and increasing series resistance; at high current density, these sites become localized Joule-heating hotspots. Voids further concentrate current and act as precursors to early interconnect failure through void growth and coalescence. The presence of a Cu_2O phase is particularly detrimental because copper oxide is electrically resistive and mechanically brittle; it prevents proper diffusion bonding and increases interface resistivity. Misalignment reduces effective pad overlap, increasing resistance and susceptibility to thermo-mechanical fatigue, while missing pads result in open circuits, leading to immediate functional failure. Edge delamination is often an indicator of non-uniform pressure distribution or CMP non-planarity, and it can propagate under thermal cycling, degrading reliability over time [12].

B. Dielectric-Dielectric Interface

At the Dielectric–Dielectric interface, edge delamination and interface delamination compromise mechanical robustness and hermetic sealing. Edge and interfacial Delaminations here reduce adhesion strength, enabling moisture ingress and facilitating corrosion at adjacent metal interfaces. Over repeated thermal cycling, this can accelerate crack initiation and propagate into conductive regions, indirectly degrading electrical performance [13].

C. Barrier Interface

Within the Barrier interaction region, protruded barrier layers represent a critical topographical defect. Barrier materials such as Ta or TiN are designed to prevent Cu diffusion into surrounding dielectrics; however, if the barrier protrudes due to CMP non-uniformity or deposition anomalies, it can physically block intimate Cu–Cu contact [14]. This results in localized non-bonded regions or increased interfacial resistance. Additionally, protrusions introduce stress concentration sites that may initiate cracks under mechanical or thermal loading.

D. Cu-Barrier Interface

At the Cu–Barrier interface, defects such as galvanic corrosion, delamination, and unintended overlap degrade both adhesion and electrical continuity. The Cu–Barrier interface must ensure low-resistance current flow while preserving diffusion blocking capability. Delamination increases interfacial resistance and can serve as a diffusion pathway, compromising long-term reliability. Overlap between Cu-Barrier may create unintended voids, current pathways, or localized geometric irregularities.

E. Cu-Dielectric Interface

The Cu–Dielectric interface is susceptible to geometric overlap anomalies. Overlap at the Cu-Dielectric interface alters the electric field distribution and local stress states, accelerating dielectric breakdown in high-field applications.

F. Cu-Dielectric Interface

At the barrier–dielectric interface, interface cracking is a critical failure mechanism. Since the barrier layer adheres to both Cu and dielectric materials, any crack formation at the barrier–dielectric interface reduces mechanical adhesion and may open diffusion pathways for copper ions. This not only compromises reliability but also increases the likelihood of time-dependent dielectric breakdown (TDDB) and leakage currents.

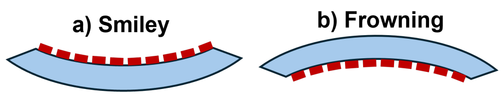

Fig. 4: Proposed cross-section workflow for hybrid bonding interface analysis.

III. Warpage and Interfacial Defect Correlation

Several studies have empirically demonstrated a correlation between warpage and interfacial defects. The apparent manifestation of warpage-related defects post-bonding is misalignment. In both D2W and W2W conditions, a degree of increase in warpage can lead to severe misalignment between Cu-Cu, which, when combined with an improper CMP process, results in direct contact between Cu-Barrier and Cu-Dielectric due to misalignment, thereby causing interfacial defects.

In one study, it was shown that top-bonded wafers with compressive stress that deform into a convex (Smiling) shape are more effective at reducing edge voids in a wafer-to-wafer bonding process than wafers with tensile stress that deform into a concave (Frowning) shape, attributed to bonding speed and the Joule-Thompson effect during bonding as mentioned in Fig. 4. These varying phenomena lead to voids and delaminations at the Cu-Cu, Cu-Dielectric, and Dielectric-Dielectric interfaces in the edge regions of the wafers and ultimately the yield loss [15].

In dielectrics, a high interfacial dielectric-dielectric bonding energy plays an important role in controlling warpage; if defects occur in this region due to improper CMP or bonding, which compromise interfacial bonding energy, it can increase warpage.

Generalizing the case with material systems such as metal, barrier, and dielectric that are interacting with an inherent CTE mismatch within their interfaces during thermal cycling process, will lead to the growth, propagation, and coalescing of the voids and delaminations within these interfaces outlined in Fig. 3, by increasing the local thermal stresses, leading to higher warpage and unpredictable deformation patterns, the residual affect from these will likely degrade the barrier layer to allow diffusion of Cu atoms into the dielectric, leading to dielectric breakdown and removing the isolation needed for two neighbouring Cu vias, the cyclic effects arising from this process ends up breaking down the interconnects.

IV. Workflow for Pre and Post Bond Evaluation

To address the critical metrology and reliability challenges associated with hybrid bonding in advanced three dimensional integration, this work proposes a unified inspection and characterization workflow that bridges pre bonding diagnostics with post bonding defect analysis. The framework is designed to establish a direct correlation between initial wafer level conditions and the eventual formation of interfacial defects, thereby enabling predictive reliability assessment.

A. Pre Bond Inspection Using Shadow Moiré Interferometry

The pre bonding stage utilizes shadow moiré interferometry as a rapid, non contact optical metrology technique to capture full field warpage distributions across the wafer surface. The primary advantage of this technique lies in its ability to generate high resolution warpage maps within seconds, making it highly suitable for inline inspection [16]. These maps provide quantitative insight into non uniformities arising from residual stresses, material mismatch, or process induced deformation. In the context of hybrid bonding, such deviations are critical, as excessive warpage can lead to non uniform contact pressure, localized air gaps, and ultimately incomplete bonding or void formation.

By establishing threshold based criteria on allowable warpage and curvature gradients, the shadow moiré measurements serve as an early stage screening mechanism. This enables the identification of high risk wafers prior to bonding, thereby reducing yield loss and preventing defect propagation into subsequent processing steps.

B. Post Bond Analysis Through Advanced Sample Preparation and SEM Imaging

Following bonding, the workflow incorporates a targeted sample preparation methodology to enable high fidelity cross sectional analysis of the bonded interface. Techniques such as precision mechanical polishing combined with localized material removal ensure minimal introduction of artifacts while exposing critical regions of interest.

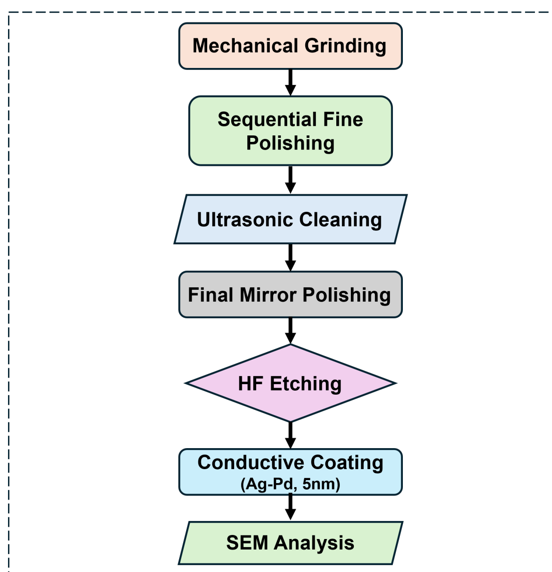

Fig. 5: Proposed cross-section workflow for hybrid bonding interface analysis.

Subsequent scanning electron microscopy imaging provides nanoscale resolution of interfacial features, including voids, unbonded regions, oxide residues, and delamination pathways. Unlike conventional inspection methods, SEM based characterization allows direct visualization of defect morphology and spatial distribution, offering valuable insights into failure mechanisms [17].

1) Sample Preparation: The proposed cross sectional metallography workflow, as illustrated in Fig. 5, enables high resolution defect characterization in advanced interconnect structures through a carefully controlled material removal sequence. The process begins with low speed mechanical grinding at 50 RPM to minimize deformation and preserve interface integrity, followed by progressive abrasive refinement using grit sizes of 600, 800, and 1200 to reduce surface roughness while maintaining micro scale feature fidelity. Subsequent polishing is performed using 6 micrometer and 3 micrometer monocrystalline diamond suspensions, each followed by ultrasonication to remove debris and prevent particle embedding. A final ultra fine polishing step with 0.05 micrometer diamond suspension and non colloidal silica produces a mirror quality surface suitable for high resolution imaging.

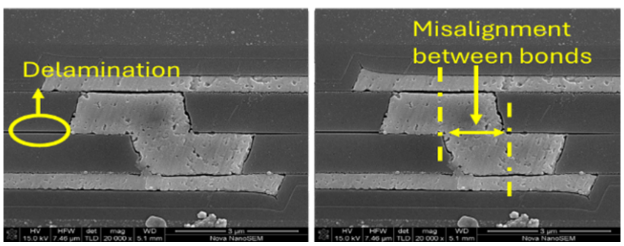

Fig. 6: Scanning electron microscopy of hybrid bonding with representative defects.

To enhance imaging contrast and mitigate electron beam induced charging, the prepared cross section is coated with a thin 5 nanometer silver palladium layer prior to scanning electron microscopy [18]. Selective chemical etching using hydrofluoric acid further delineates material interfaces, enabling clearer visualization of layer boundaries. The resulting SEM analysis provides detailed insight into the internal structure, allowing precise identification of defects such as interconnect voids. The observed results confirm that the workflow effectively exposes sub surface defects, demonstrating its suitability for reliability driven characterization of advanced packaging architectures.

2) Analysis After Sample Preparation: The scanning electron microscopy images shown in Fig. 6 reveal several critical interfacial defects that directly impact the integrity and reliability of hybrid bonding structures. The bonding interface exhibits non uniform contact, irregular morphology, and localized discontinuities, indicating deviations from ideal planar bonding conditions. These features highlight the sensitivity of the bonding process to local geometric variations and alignment precision, particularly at fine pitch dimensions [19]. A key defect observed is interfacial delamination, appearing as localized regions of separation with distinct contrast variations that indicate weak adhesion. These regions are predominantly concentrated near bonding edges, suggesting stress accumulation and non uniform load distribution, which can act as initiation sites for crack propagation under thermal and mechanical loading [20].

In addition to delamination, the images reveal lateral misalignment between bonding features, where interconnects are offset relative to corresponding pads, resulting in reduced effective contact area and asymmetric interfaces [21]. This misalignment introduces localized stress concentrations and non uniform current distribution, potentially degrading electrical performance through increased resistance and susceptibility to electromigration. Furthermore, interfacial gaps and void like features are evident as dark contrast regions, indicating incomplete bonding and disrupted material continuity. These voids compromise both mechanical strength and electrical pathways, serving as stress concentration sites that accelerate degradation under thermo mechanical cycling, thereby emphasizing the importance of precise alignment and uniform bonding conditions in advanced interconnect technologies.

V. Pre-Bond Warpage Metrology and Screening for Hybrid Bonding Reliability

To mitigate the bonding defects observed in Fig. 3, a pre-bond metrology checkpoint was introduced to screen the substrates for excessive out-of-plane deformation (bow) prior to wafer bonding. The primary origin of the observed defects is substrate non-planarity accumulated during the thermal budget. Because the substrate is Si while the bonding material is Cu, the coefficient of thermal expansion (CTE) mismatch generates thermomechanical stress during heating/cooling cycles, which establishes as global bow and, in some cases, diagonal curvature across the sample. Excessive bow reduces the effective contact area at bond initiation, leads to non-uniform local contact pressure, and increases susceptibility to void formation and unbonded regions during the subsequent hybrid bonding step.

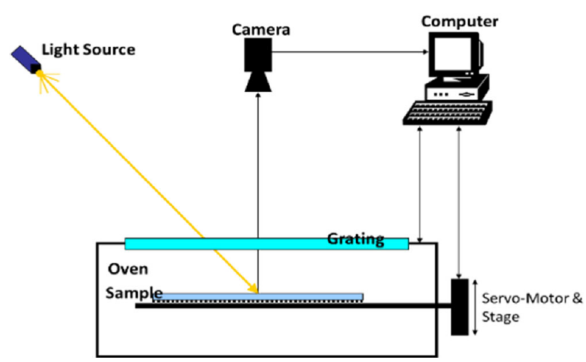

Fig. 7: Schematic of the principle of out of plane deformation measurement in the system

Bow measurements were performed on nine 1 in × 1 in coupons using a commercial shadow moiré metrology tool (Akrometrix Inc.). The shadow moiré method provides a full-field height/displacement map by forming moiré fringes from a reference grating and the deformed specimen surface. As schematically illustrated in Fig. 7, the specimen is illuminated through a mechanical grating, producing fringe contours that correspond to loci of constant out-of-plane displacement.

A camera captures the fringe pattern, while a servo-driven translation stage introduces controlled phase shifts between the grating and the specimen [22]. This phase-shifting procedure enables sub-fringe interpolation, thereby improving spatial resolution and enhancing the accuracy of the reconstructed height field compared to single-image fringe interpretation.

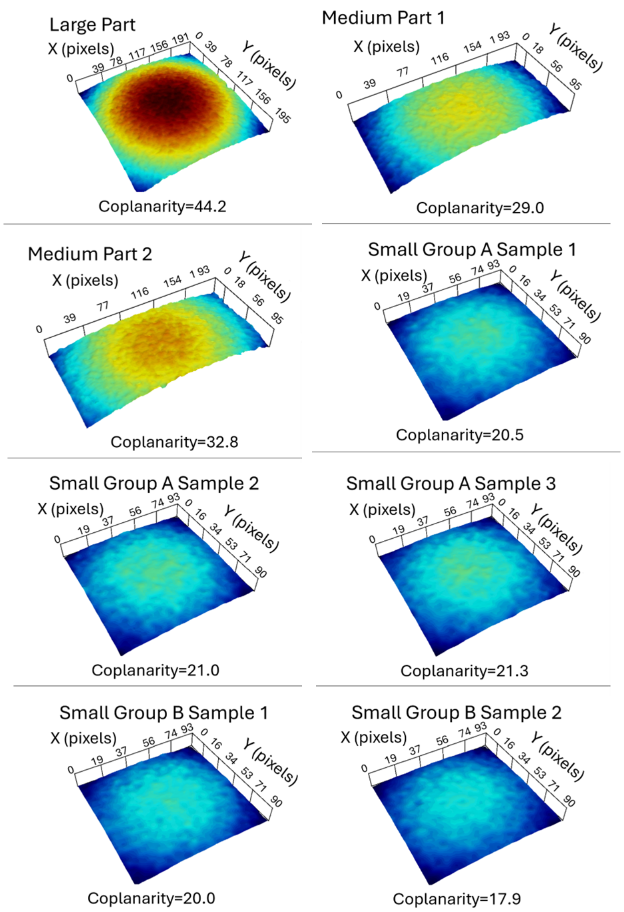

Fig. 8: Coplanarity of the bowed wafers

Using the reconstructed out-of-plane displacement maps, the bow of each coupon was extracted and used as a quantitative measure of coplanarity shown in Fig. 8. In addition to reporting the overall bow magnitude, diagonal mean profiles (both upward and downward diagonals) were evaluated across each coupon, as shown in Fig. 9, to capture curvature modes that may not be fully represented by a single global metric. These diagonal trends provide a consistent basis to compare curvature directionality and identify coupons exhibiting asymmetric or saddle-like deformation that can be particularly detrimental to uniform bonding [23]. The measured bow values were compared against the allowable limit specified by the bonding equipment/materials manufacturer. Coupons exceeding the manufacturer-defined bow tolerance were classified as unsuitable for the subsequent hybrid bonding process, whereas coupons within specification were advanced to bonding. This pre-screening step reduces the probability of bonding non-uniformities and directly addresses the defect mechanisms associated with thermally induced curvature.

VI. Predictive Reliability Modeling Framework

The proposed predictive reliability framework establishes a quantitative linkage between pre-bond wafer warpage characteristics and post-bond interfacial defect formation by integrating metrology-derived deformation features with defect occurrence statistics. The framework is designed to shift hybrid bonding reliability assessment from a reactive inspection-based approach to a predictive data-driven methodology that supports wafer screening, process optimization, and yield estimation.

The warpage state of a wafer is represented as a spatial out-of-plane deformation field $W(x, y)$ obtained from full-field shadow moiré interferometry. From $W(x, y)$, a set of warpage descriptors is extracted, including the global bow B, local curvature $\kappa(x, y)$, curvature gradients $\nabla\kappa(x, y)$, and diagonal asymmetry metrics derived from principal deformation directions. These descriptors capture both the magnitude and spatial non-uniformity of wafer deformation, which governs contact non-uniformity during bond initiation and contributes to void nucleation, incomplete bonding, and interfacial delamination.

To quantify defect formation risk, a probabilistic defect model is defined where the likelihood of observing a defect at location (x, y) depends on local deformation and thermomechanical driving forces:

$$P_{\text{defect}}(x, y) = f\big(W(x, y),\, \kappa(x, y),\, \sigma_{\text{CTE}},\, \Delta T,\, \gamma_{\text{bond}}\big) \tag{1}$$

where σ_{CTE} denotes the thermomechanical stress induced by coefficient of thermal expansion mismatch, ΔT is the applied thermal budget, and γ_{bond} represents the effective bonding energy that governs interfacial adhesion. Regions exhibiting high curvature or steep curvature gradients are expected to experience reduced effective contact area and non-uniform local pressure, increasing susceptibility to warpage-driven bonding defects.

For practical implementation, the wafer is discretized into spatial bins, and a scalar risk score is computed for each region i using a linearized surrogate model:

$$R_i = \alpha B_i + \beta \kappa_i + \gamma \left\| \nabla \kappa_i \right\|, \tag{2}$$

where α, β, and γ are weighting coefficients calibrated using experimentally observed defect statistics from post-bond cross-sectional scanning electron microscopy. The risk score enables classification of wafer regions into low-, moderate-, and high-risk zones, supporting targeted screening and process control.

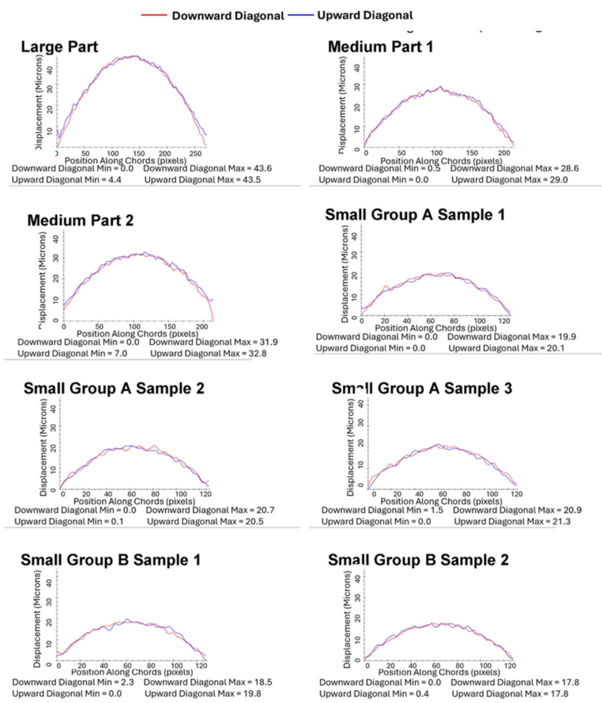

Fig. 9: Diagonal wafer bow profiles derived from full field warpage measurements

To extend the framework to yield prediction, the expected defect density D is estimated by integrating defect probability across the bonding area:

$$D = \iint_{\Omega} P_{\text{defect}}(x, y)\, \mathrm{d}x\, \mathrm{d}y, \tag{3}$$

where Ω denotes the effective bond region. A defect-limited yield estimate can then be obtained using a Poisson yield model:

$$Y = \exp(-D\, A) \ \ or\ \ Y = e^{(-DA)} \tag{4}$$

where A is the effective bonding area. This formulation provides a direct pathway to estimate yield and reliability risk using only pre-bond metrology features, thereby reducing reliance on destructive post-bond analysis.

The framework is compatible with machine learning extensions in which warpage features extracted from $W(x, y)$ form the input vector and defect classes defined by the interfacial taxonomy serve as labels. This enables nonlinear mapping between deformation signatures and defect outcomes across multiple interface types, including Cu–Cu, dielectric–dielectric, and heterogeneous material interfaces. Overall, the proposed framework unifies pre-bond inspection and post-bond reliability assessment into a predictive pipeline that supports early identification of high-risk wafers, improved process control, and enhanced yield in advanced three-dimensional integration systems.

VII. Conclusion and Future Directions

This work establishes a predictive reliability framework that correlates pre bond wafer warpage with post bond interfacial defect formation in hybrid bonding systems. By integrating full field shadow moiré metrology with high resolution scanning electron microscopy, the study demonstrates that deformation driven non uniformities directly influence defect mechanisms such as voids, delamination, and misalignment. We developed a structured defect taxonomy across multiple interfaces that enables systematic classification and strengthens root cause analysis. We developed a model that utilizes warpage descriptors to quantify defect risk and estimate yield through a probabilistic formulation. Our framework provides a scalable pathway toward data driven process optimization and reliability prediction. Future work will focus on machine learning integration, real time metrology feedback, and extension toward layout level and process aware reliability modeling for advanced three dimensional integration systems.

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