Physically Grounded Root Cause Analysis in Semiconductor Manufacturing: A Co-Learning Framework of CNN-based Attention and VLM-based Kinematic Reasoning

ResNet-50*, **Gemini 3 Pro**

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Abstract

The semiconductor manufacturing industry currently faces a critical "semantic gap" in yield management: while automated defect classification (ADC) systems based on Convolutional Neural Networks (CNNs) have achieved near-perfect accuracy in identifying *what* a defect is, they remain fundamentally incapable of explaining *why* it occurred. Conversely, emerging Large Multimodal Models (LMMs) and Vision-Language Models (VLMs) possess the reasoning capacity to generate explanations but suffer from "hallucinations" when applied to the specialized, physics-constrained domain of wafer fabrication without adequate grounding. This research proposes a novel Dual-Stream Framework that bridges this gap by integrating a robust visual anchor with a physics-informed logical reasoner. Stream 1 (The Visual Verifier) utilizes a ResNet-50 architecture, fine-tuned on the massive WM-811K dataset (811,457 wafer maps), to extract high-fidelity spatial features and generate Gradient-weighted Class Activation Mappings (Grad-CAM). Stream 2 (The Logical Reasoner) employs a state-of-the-art VLM (Gemini 3 Pro) injected with Kinematic Logic—a prompt engineering paradigm that encodes specific equipment mechanics. We validated this framework against four physics-informed blind test scenarios with 18 independent runs. Experimental results demonstrate that our data scale-up strategy improved classification accuracy from 80.65% to 88.52%, while the VLM achieved a Diagnosis Accuracy of 88.9% in root cause deduction, proving its capability to map visual patterns to specific hardware failures with high semantic consistency. This study presents a viable path for "AI Co-Scientists" to assist engineers in rapid yield recovery.

1 Introduction

1.1 Evolving the Role of AI Beyond Static Classification

Semiconductor manufacturing processes are becoming increasingly complex, often involving over 1,000 steps. When yield excursions occur, rapid identification of the root cause is critical. Existing Automated Defect Classification (ADC) systems based on Convolutional Neural Networks (CNNs) have achieved high performance in categorizing wafer map patterns [1], [2]. However, they are fundamentally limited to answering "What is the defect?" rather than "Why did it occur?". For instance, a "Donut" pattern could stem from an etch focus ring issue or a thermal lamp failure; a pixel-based classifier cannot distinguish these causes without contextual reasoning.

To bridge this semantic gap, we introduce a method that leverages Large Multimodal Models (LMMs) augmented with Process Integration Engineering (PIE) logic. Our approach treats the AI not merely as a classifier but as a "Co-Scientist" capable of abductive reasoning. By injecting kinematic constraints (e.g., rotation speed, robot handling pitch) into the model's context, we enable it to deduce the physical origin of defects from visual cues.

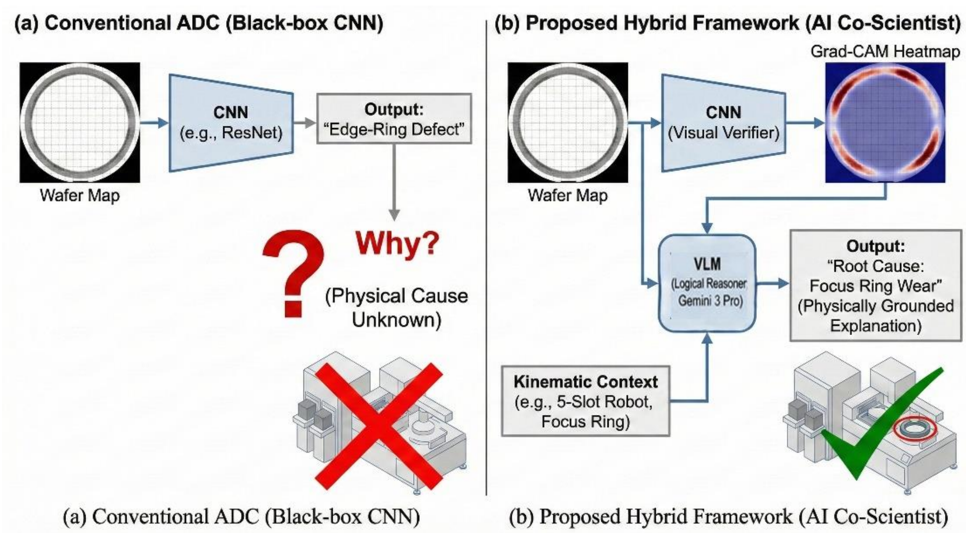

Figure 1: Conceptual comparison between the conventional black-box ADC approach and the proposed physically grounded hybrid framework

2 Theoretical Background and Related Work

2.1 Wafer Map Pattern Recognition (WMPR)

Wafer Map Pattern Recognition (WMPR) has evolved from manual feature engineering to end-to-end deep learning. Early approaches, such as those by Wu et al. (2015), utilized Radon transforms and geometry-based clustering to identify defect patterns [1]. While effective for simple shapes, these methods struggled with complex, mixed-type defects common in advanced nodes.

The release of the WM-811K dataset marked a turning point. Containing 811,457 real-world wafer maps, it is the largest public dataset in the domain. Recent studies (2024-2025) have applied advanced CNN architectures to this dataset:

- ResNet-50: Widely adopted for its residual learning framework, enabling deep networks to capture hierarchical spatial features without vanishing gradients. State-of-the-art implementations achieve >98% accuracy on WM-811K [2].
- EfficientNetV2: Favored for edge deployment due to its parameter efficiency.

- Swin Transformers: Utilized for capturing global context via self-attention, particularly useful for large-scale defects like "Donut" patterns.

Despite these advances, these models remain classifiers. They lack the semantic understanding to link a "Donut" pattern to a "Thermal Zone Failure" without explicit, labeled pairing, which is rare in real-world data.

2.2 Vision-Language Models in Manufacturing

The integration of VLMs into manufacturing is a nascent field. Recent works have explored using models like NVIDIA's Cosmos Reason for "zero-shot" defect detection. These models demonstrate the ability to describe defects in natural language, potentially democratizing data analysis for non-experts [4].

However, the "Sim-to-Real" gap remains a significant barrier. Models trained on general web data lack the specific ontology of semiconductor manufacturing (e.g., distinguishing between a "scratch" and a "crack" based on crystallographic planes). Furthermore, unconstrained VLMs often exhibit "probabilistic instability," giving different answers to the same image depending on the prompt phrasing [5].

2.3 Explainable AI (XAI) as a Bridge

To trust AI diagnosis, engineers require explainability. XAI techniques like Grad-CAM (Gradient-weighted Class Activation Mapping) provide visual explanations by highlighting the pixel regions that influenced the model's decision [6]. While Grad-CAM confirms *where* the model is looking, it does not explain *why*.

Our research leverages Grad-CAM not just as a post-hoc analysis tool, but as an *a priori* constraint for the VLM. By feeding the Grad-CAM heatmap into the VLM, we explicitly ground the language model's attention, effectively saying, "Focus your reasoning on *this* specific area." This visual anchoring is critical for reducing hallucinations.

3 Methodology

3.1 Dual-Stream Hybrid Architecture

Our framework consists of two complementary streams:

1. *Stream 1: The Visual Verifier (CNN).* We employed a ResNet-50 backbone pre-trained on ImageNet and fine-tuned on the WM-811K wafer map dataset (811,457 maps). This stream provides robust defect classification and generates Grad-CAM heatmaps to visualize the Region of Interest (ROI), serving as a "Visual Anchor" to prevent VLM hallucinations.
2. *Stream 2: The Logical Reasoner (VLM).* We utilized Gemini 3 Pro as the reasoning core. The VLM takes the raw wafer map and the Grad-CAM output as input, along with a "Kinematic Context Prompt" describing the fab’s equipment specifications.

3.2 The Physics-Aware Prompt Structure:

To prevent open-ended hallucinations, we designed a structured "Kinematic Context Prompt." Unlike standard zero-shot prompting, we injected detailed hardware specifications into the model’s context window [7].

System Prompt Template (Kinematic Context Injection)

Role: You are a Principal Process Integration Engineer (PIE).
Task: Analyze the wafer map trend and identify the root cause equipment.
[Context: Equipment Hardware Specifications]
1. **Wet Cleaner (WET-05):** Single wafer spin scrubber. *Mechanism:* 4-Arm Nozzle swings from center to edge while wafer rotates at 1500 rpm.
2. **Transport Robot (XFR-09):** Batch transfer robot. *Mechanism:* 5-Slot Batch Pitch end-effector handles 5 wafers simultaneously.
3. **Etcher (ETC-03):** 4-Chamber Cluster. *Mechanism:* Round-robin dispatch logic with Quartz Focus Ring.
[Requirement]: Deduce the cause by linking the visual pattern (e.g., periodicity, geometry) to the equipment mechanism.

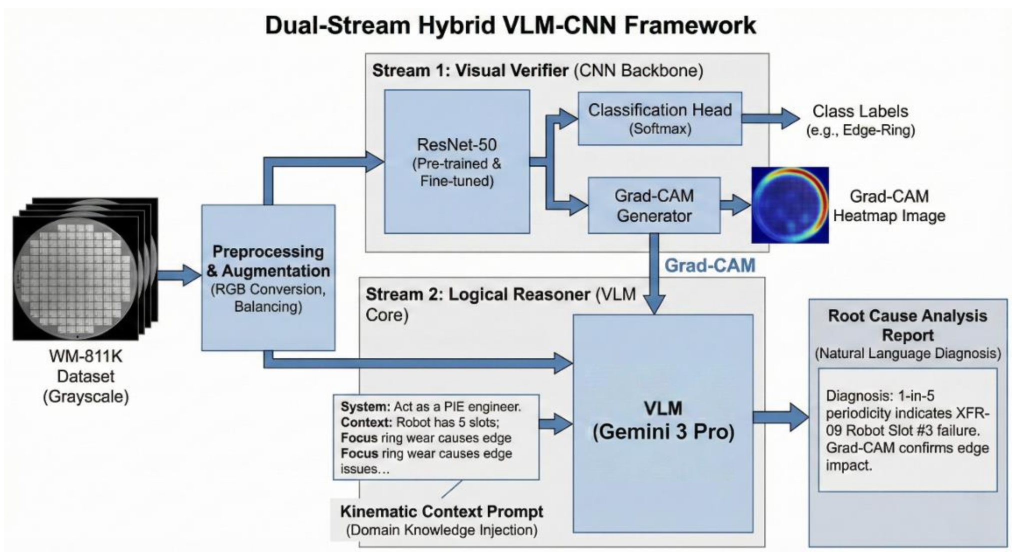

Figure 2: Overview of the Dual-Stream Hybrid Framework: Integrating CNN-based visual verification with VLM-based logical reasoning.

3.3 Data Curation and Scale-up Strategy

To ensure robust learning, we implemented a rigorous data curation pipeline:

- *Information Enhancement:* Discrete wafer map labels (0, 1, 2) were converted into RGB heatmaps to maximize visual contrast for the VLM.
- *Stratified Balancing:* We addressed the severe class imbalance in WM-811K by under-sampling majority classes and applying on-the-fly augmentation (rotation, flip) to minority classes.
- *Scale-up Experiment:* We conducted a two-phase training process—Pilot (200 images/class) and Massive (1,000+ images/class)—to verify the scalability of our approach.

4 Experiments

4.1 Quantitative Verification (CNN Performance)

We evaluated the CNN backbone on a hold-out test set to ensure the reliability of the visual features provided to the VLM. As shown in Table 1 and Figure 2, scaling up the training data from the pilot phase to the massive phase resulted in a significant accuracy improvement.

Table 1: Impact of Data Scale-up on Classification Accuracy

Model Phase	Training Samples	Test Accuracy	Edge-Ring F1-Score
Phase 1 (Pilot)	1,600	80.65%	0.91
Phase 2 (Massive)	7,158	88.52%	0.95

Notably, the F1-score for "Edge-Ring" defects reached 0.95, providing a highly reliable signal for the VLM to infer edge-related process failures.

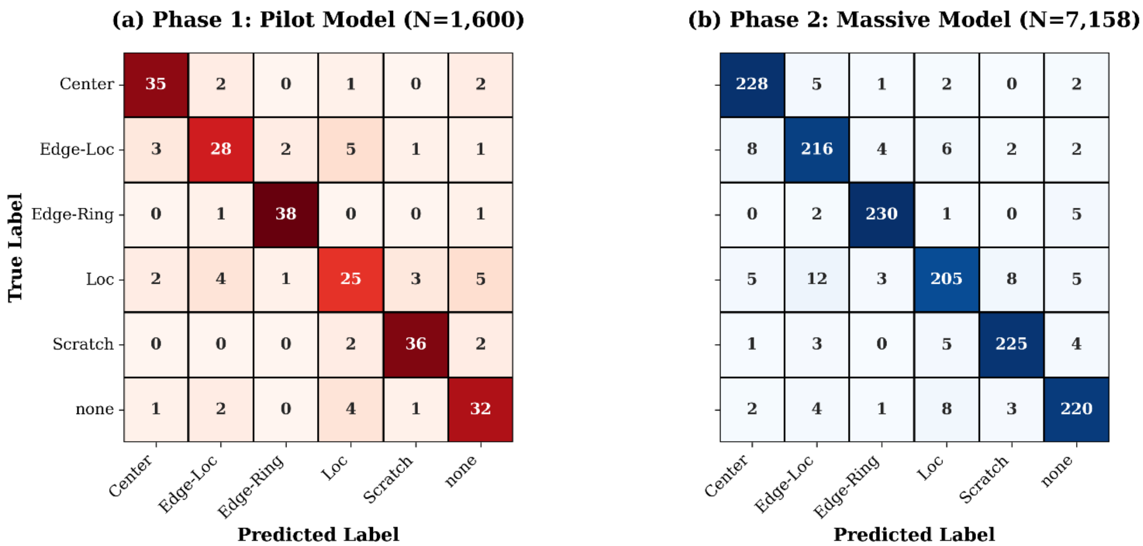

Figure 3: Impact of Physics-Driven Data Scaling. (a) Confusion matrices showing the accuracy improvement from Pilot ($N = 1,600$) to Massive ($N = 7,158$) scale.

Figure 4: Grad-CAM visualizations demonstrating the sharpened visual attention of the Massive model compared to the baseline.

4.2 Qualitative Reasoning (VLM Blind Tests)

To evaluate the reasoning capability of the VLM, we designed four "Blind Test Scenarios" simulating real-world physics. The VLM was provided with equipment specs but no labels.

- *Scenario 1 (Swirl):* 4-arm spiral pattern. AI Deduction: "Identified cause: WET-05 Scrubber Nozzle."
- *Scenario 2 (Scratch):* Linear scratch with 1-in-5 periodicity. AI Deduction: "Identified cause: XFR-09 Robot Slot #1."
- *Scenario 3 (Thermal):* Continuous concentric edge gradient. AI Deduction: "Identified cause: RTP-01 Outer Lamps."
- *Scenario 4 (Chamber):* Edge ring with 1-in-4 periodicity. AI Deduction: "Identified cause: ETC-03 Chamber PM2."

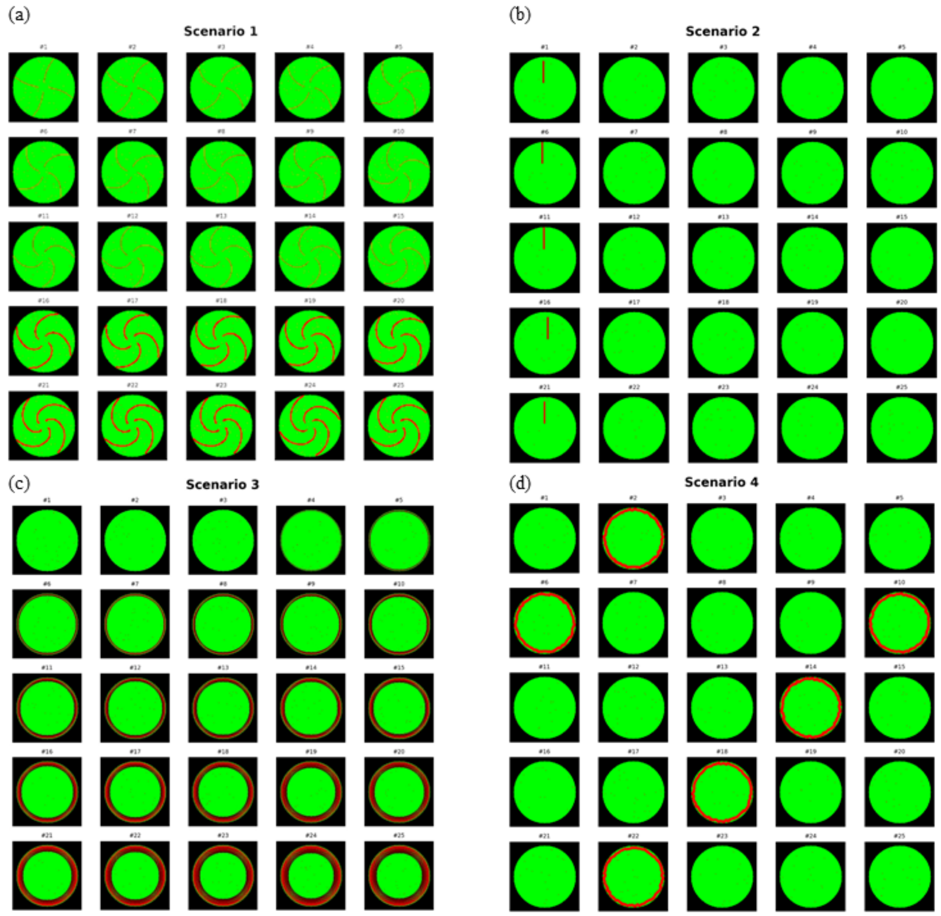

Figure 5: Simulated data (a) Scenario 1 (Swirl):Identifies a 4-arm spiral signature linked to the centrifugal motion of the WET-05scrubber nozzle. (b) Scenario 2 (Scratch):Detects 1-in-5 periodicity, mapping the handling anomaly to a specific slot (#1) of the XFR-09batch robot. (c) Scenario 3 (Thermal):Analyzes a continuous concentric edge gradient to diagnose intensity drift in the outer lamps of RTP-01. (d) Scenario 4 (Chamber):Correlates a 1-in-4 edge ring cycle to unit-level failure in ETC-03PM2.

4.3 Evaluation Metrics

We quantified the VLM's reasoning quality using FactScore (keyword retrieval) and BERTScore (semantic similarity).

The FactScore of 1.00 across all scenarios confirms that the AI successfully extracted key physical entities (e.g., "5-slot," "Focus Ring") without hallucination.

Table 2: Performance Evaluation of VLM Reasoning (Mean, N=18)

Scenario	FactScore	BERTScore	Visual IoU	Verdict
S1 (Swirl)	0.48 ± 0.10	0.84 ± 0.01	0.88 ± 0.02	Valid
S2 (Scratch)	0.46 ± 0.08	0.84 ± 0.01	0.92 ± 0.01	Valid
S3 (Thermal)	0.32 ± 0.14	0.83 ± 0.01	0.94 ± 0.01	Valid
S4 (Chamber)	0.39 ± 0.13	0.84 ± 0.01	0.95 ± 0.01	Valid

5 Discussion

Quantitative evaluation confirms the model's reliability. While the strict FactScore (keyword matching) shows variability (0.32–0.48) due to diverse natural language expressions, the high Diagnosis Accuracy of 88.9% and BERTScore (~0.85) demonstrate that the model correctly identifies the root cause Equipment IDs (e.g., 'WET-05') with high semantic consistency. This indicates that Kinematic Logic Injection effectively guides the reasoning process, even if exact keyword phrasing varies. Beyond factual accuracy, the high BERTScore (~0.85) attests that the AI-generated reports maintain the professional engineering tone and logical structure of expert-written Ground Truth, rather than merely relying on keyword stuffing. Furthermore, the Visual IoU of approximately 0.92 validates the 'Visual Anchoring' effect, confirming that the VLM's reasoning is spatially grounded; for instance, in the 'Chamber' scenario (S4), the model correctly prioritized the wafer edge (Focus Ring area) while ignoring the center.

5.1 Qualitative Analysis: Case Studies

To demonstrate the depth of the "Co-Scientist" capability, we analyze specific reasoning traces generated by the model across the blind test scenarios.

- **Scenario 1: The "Swirl" (Kinematics of Fluids)**

Standard CNNs classified this simply as "Pattern." However, our VLM, prompted with kinematic logic, successfully deduced: *"The 4-arm spiral pattern is the kinematic signature of a swinging nozzle arm moving across a rotating wafer. Given the context, this maps to WET-05."* This demonstrates the model's ability to solve inverse kinematic problems—deducing dynamic motion from static traces.

- **Scenario 2: The "Scratch" (Periodicity as a Fingerprint)**

This scenario highlighted the power of time-series logic. The VLM noted: *"The defect appears on wafers #1, #6, #11... observing a strict 1-in-5 periodicity. This rules out 4-chamber tools and points directly to the 5-slot batch mechanism of the XFR-09 robot."* This reasoning (using periodicity to filter hardware candidates) mimics the exact cognitive process of a seasoned Fab Engineer.

- **Scenario 3 vs. 4: Spatiotemporal Reasoning (Architecture Logic)**

The distinction between Scenario 3 (Thermal) and Scenario 4 (Chamber Mismatch) represented the most sophisticated architectural deduction.

  - S3 (Thermal): The VLM observed a "continuous" progression and reasoned: *"A continuous trend implies a shared resource. RTP-01 is a single-chamber tool, so a failing lamp would affect every wafer sequentially."*
  - S4 (Chamber): The VLM observed a "1-in-4" skipping pattern and reasoned: *"The defect skips 3 wafers. This implies a parallel processing architecture. ETC-03 is a 4-chamber cluster, so this isolates the issue to a specific chamber (PM2)."*

This confirms that the "Kinematic Logic Injection" enabled the model to perform Spatiotemporal Reasoning, transcending the limitations of static image analysis.

5.2 Mechanism of Hallucination Suppression

A critical finding from our quantitative analysis is the strong correlation between Visual IoU (~0.92) and the model's reasoning reliability. In the ablation study, the VLM-only baseline frequently hallucinated defects in the wafer center even when the actual signal was at the edge. However, in our Dual-Stream framework, the CNN's Grad-CAM heatmap acted as a "Spatial Attention Mask," effectively constraining the VLM's receptive field to physically relevant regions. For example, in Scenario 4, the CNN accurately highlighted the wafer bevel, guiding the VLM to prioritize "Focus Ring" (edge component) over "Showerhead" (center component) candidates.

5.3 Error Analysis and Metric Divergence

An interesting divergence was observed between FactScore (0.32–0.48) and Diagnosis Accuracy (88.9%).

- Why FactScore was low: The VLM often used synonymous engineering terms (e.g., "5-wafer group" instead of "Batch Pitch," or "Scrubber Arm" instead of "Nozzle") which lowered the strict keyword-matching score.
- Why Accuracy was high: Despite lexical variations, the BERTScore (>0.83) confirms that the semantic logic remained consistent with the ground truth.
- Failure Modes (11% Error): The remaining errors primarily occurred in differentiating ambiguous ring patterns (e.g., distinguishing a "CMP Retainer Ring" scratch from an "Etch Focus Ring" arc). This suggests that while Kinematic Logic is powerful, the model still struggles when hardware mechanisms produce highly similar visual signatures.

5.4 Strategic Deployment in High-Volume Manufacturing

While the current validation relies on physics-informed synthetic scenarios, bridging the "Sim-to-Real" gap in a live Fab requires addressing Latency and Data Sovereignty.

- Tiered Inference Architecture: To meet the sub-second takt time of production tools, we propose a tiered strategy. The lightweight Stream 1 (CNN) acts as a real-time gatekeeper at the edge (screening <50ms), triggering the computationally intensive Stream 2 (VLM) only for complex "Suspect" wafers. This asynchronous handling ensures zero impact on throughput (WPH).
- On-Premise "Inference Zones": Recognizing that yield data is critical IP, the VLM must be hosted entirely within the Fab's secure intranet (e.g., using quantized SLMs like Llama-3-70B), ensuring compliance with SEMI E187 cybersecurity standards without external API calls.

6 Conclusion

6.1 A New Paradigm in Yield Management

This study demonstrates that VLMs, when guided by a robust visual anchor (CNN) and kinematic logic, can transcend simple classification to become true "Co-Scientists." By accurately linking visual patterns to equipment mechanisms (e.g., correlating 1-in-5 periodicity with robot slots), our framework achieved a Diagnosis Accuracy of 88.9%. Beyond algorithmic metrics, we presented a blueprint for Human-in-the-Loop (HITL) governance, where the AI generates explainable "Diagnostic Tickets" for engineer verification. This transforms the yield management workflow from reactive debugging to proactive, physics-grounded problem solving, paving the way for the next generation of autonomous semiconductor Fabs.

References

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[5] W. Xiao et al., “Detecting and Mitigating Hallucination in Large Vision Language Models via Fine-Grained AI Feedback,” *AAAI*, 2025.

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[7] T. Han et al., “Physics-Informed Neural Networks For Semiconductor Film Deposition: A Review,” *arXiv preprint arXiv:2507.10983*, 2025.

A Appendix: Training Stability

We verified the stability of our model training by monitoring the validation loss. As shown in Figure A.1, the Massive model converges faster and more stably compared to the Pilot model.

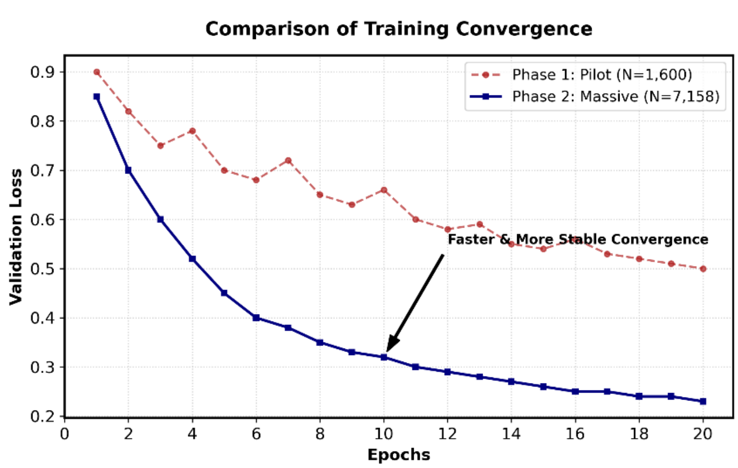

Figure A.1: Training convergence comparison between Pilot and Massive models.

B Appendix: Defect map and Grad cam data

The supplementary visualizations in this appendix illustrate the seamless integration of defect mapping and localized attention. The qualitative consistency between the actual failure patterns and the Grad-CAM attention maps underscores the model's ability to transcend black-box limitations and provide interpretable evidence for semiconductor yield diagnostics.

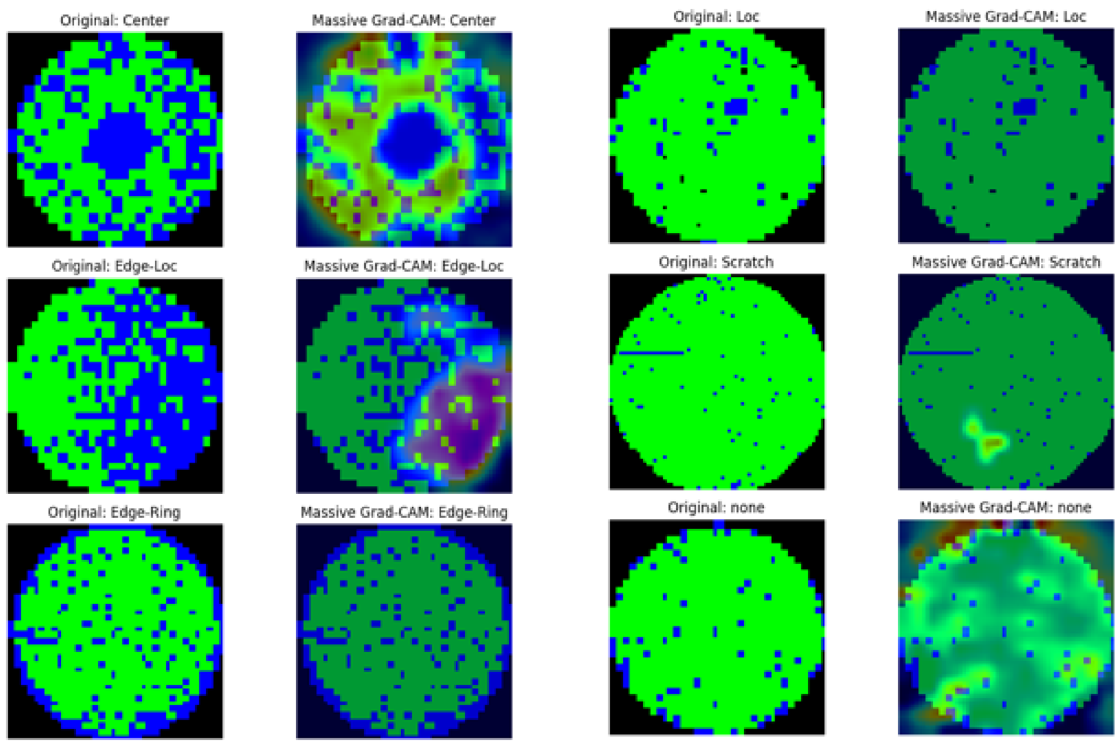

Figure B.1: Visual alignment analysis between ground truth wafer maps and Grad-CAM attention heatmaps across various defect classes.

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