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Adaptive Fault Diagnosis in Wafer Production Lines Fusing Knowledge Graphs and Deep Reinforcement Learning

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Abstract

The semiconductor manufacturing industry faces increasing challenges in maintaining high yield rates due to the extreme complexity of modern wafer production processes. As fabrication technologies scale down to nanometer levels, the interactions between processing tools, sensor readings, and production recipes become highly non-linear and stochastic. Traditional fault diagnosis methods, ranging from statistical process control to standard supervised deep learning, often struggle with the dynamic nature of production environments and the lack of interpretability in diagnostic decisions. This paper proposes a novel framework that fuses Knowledge Graphs with Deep Reinforcement Learning to establish an adaptive, explainable fault diagnosis system. We construct a dynamic knowledge graph that semantically models the topology of the production line, capturing causal relationships between equipment, process parameters, and defect classes. Subsequently, a Deep Reinforcement Learning agent is designed to navigate this graph, learning optimal diagnostic paths to identify root causes efficiently. By treating fault diagnosis as a sequential decision-making process over a structured knowledge base, our approach not only improves diagnostic accuracy but also adapts to concept drift caused by recipe changes or equipment wear. Experimental results demonstrate that the proposed method significantly outperforms baseline approaches in both precision and adaptability, offering a robust solution for Industry 4.0 semiconductor foundries.

Keywords: *Wafer Manufacturing, Knowledge Graphs, Deep Reinforcement Learning, Fault Diagnosis*

INTRODUCTION

The global demand for high-performance computing and microelectronics has placed immense pressure on semiconductor foundries to maximize throughput while minimizing defect rates. Wafer fabrication is arguably one of the most complex manufacturing processes in existence, involving hundreds of sequential steps such as photolithography, etching, deposition, and chemical mechanical planarization. In such a high-stakes environment, a single excursion or equipment fault can lead to significant yield loss, costing manufacturers millions of dollars in scrapped inventory. Consequently, the rapid and accurate diagnosis of faults is paramount to operational efficiency and economic viability [1]. The transition toward Industry 4.0 and Smart Manufacturing has flooded production lines with sensors, generating terabytes of multivariate time-series data and log files daily. While this data availability presents an opportunity for advanced analytics, it also creates a bottleneck; the heterogeneity and volume of data often overwhelm traditional analytical tools. Historically, Fault Detection and Classification (FDC) systems relied heavily on univariate Statistical Process Control (SPC). While effective for detecting simple limit violations, SPC lacks the capability to model complex, multi-variable correlations that define modern process failures. More recently, data-driven approaches utilizing machine learning, particularly Deep Learning (DL), have gained prominence. Convolutional Neural Networks (CNNs) and Recurrent Neural Networks (RNNs) have shown remarkable success in classifying defect patterns from wafer bin maps and sensor streams [2]. However, these black-box models suffer from two critical limitations. First, they lack interpretability; knowing that a wafer is defective is less valuable than knowing which specific chamber or parameter caused the defect. Second, they are generally static; when a production recipe changes—a frequent occurrence in high-mix foundries—supervised models often require extensive retraining or fine-tuning, leading to periods of suboptimal performance known as catastrophic forgetting [3]. To address these challenges, this research introduces a hybrid paradigm that synergizes the structural reasoning capabilities of Knowledge Graphs (KGs) with the adaptive decision-making power of Deep Reinforcement Learning (DRL). A Knowledge Graph provides a structured representation of the manufacturing domain, linking disparate data entities—such as tool IDs, sensor parameters, and maintenance logs—through semantic relationships. This graph structure inherently supports explainability, allowing engineers to trace the logic behind a diagnosis [4]. By overlaying a DRL agent onto this graph, we transform the static retrieval of information into a dynamic search problem. The agent learns to navigate the relations within the graph to pinpoint the root cause of a fault, optimizing its policy based on feedback from diagnostic success. The primary contribution of this paper is a unified framework that enables adaptive fault diagnosis. Unlike static classifiers, our DRL agent continuously updates its understanding of the environment. When a new tool is added or a process recipe is altered, the underlying Knowledge Graph is updated, and the agent explores these new pathways, rapidly converging on updated diagnostic policies without the need for massive labeled datasets typical of supervised retraining. This adaptability is critical for modern fabs where flexibility is as important as precision [5]. Furthermore, by grounding the learning process in a semantic graph, the system provides a transparent audit trail of the diagnostic process, bridging the gap between algorithmic performance and human trust.

2. Literature Review

The domain of fault diagnosis in semiconductor manufacturing has evolved from manual inspection to sophisticated automated systems. This section reviews relevant literature in data-driven diagnosis, the application of knowledge graphs in industry, and the emergence of reinforcement learning for process control.

2.1 Data-Driven Fault Diagnosis in Semiconductor Manufacturing

The standard approach to modern fault diagnosis involves analyzing sensor data collected during the wafer processing cycle. Early implementations utilized Principal Component Analysis (PCA) and Partial Least Squares (PLS) to reduce the dimensionality of sensor data and identify outliers. While computationally efficient, these linear methods often fail to capture the complex non-linear relationships inherent in plasma etching or deposition processes [6]. As computational power increased, the industry shifted toward non-linear machine learning models. Support Vector Machines (SVMs) and Random Forests became standard for classifying fault types based on feature-engineered inputs. With the advent of deep learning, researchers began applying Convolutional Neural Networks (CNNs) to Wafer Bin Maps (WBMs) to identify spatial defect patterns, such as scratches or center rings, which correlate to specific equipment failures. Simultaneously, Long Short-Term Memory (LSTM) networks have been employed to analyze temporal dependencies in sensor time-series data. Despite their high accuracy, these deep learning models are fundamentally data-hungry and prone to overfitting when fault samples are rare, a common scenario in mature fabs where defects are minimized [7]. Moreover, purely data-driven models often ignore the physical topology of the factory. They treat correlations as causation without understanding the mechanical connectivity between a gas flow controller and a reaction chamber, leading to spurious correlations and false alarms [8].

2.2 Knowledge Graphs in Industrial AI

Knowledge Graphs have emerged as a powerful tool for organizing industrial data, moving beyond relational databases to graph-based structures that emphasize the relationships between entities. In the context of manufacturing, a KG can model the hierarchy of a factory, mapping the relationships between a specific product line, the tools used, the sensors installed on those tools, and the maintenance history of those components. Previous studies have demonstrated the utility of KGs for cognitive manufacturing, enabling systems to answer complex queries regarding production lineage and resource allocation [9]. In fault diagnosis specifically, KGs serve as a repository of expert knowledge and historical failure modes. For instance, ontology-based reasoning has been used to infer potential failure causes by traversing the relationships between observed symptoms and known fault mechanisms. However, traditional KG-based diagnosis often relies on static rule-based inference or simple path-finding algorithms, which may not scale well when the graph becomes massive and the relationships become probabilistic rather than deterministic [10]. The integration of learning algorithms with graph structures, known as Graph Representation Learning, has shown promise in predicting missing links or classifying nodes, but the application of these techniques to real-time decision-making in wafer production remains under-explored [11].

2.3 Deep Reinforcement Learning for Adaptive Control

Reinforcement Learning (RL) differs from supervised learning by focusing on sequential decision-making to maximize a cumulative reward. In the industrial sector, RL has been primarily applied to robotic control and supply chain optimization. Deep Reinforcement Learning (DRL), which utilizes deep neural networks to approximate value functions or policies, allows agents to handle high-dimensional state spaces. Recent work has explored DRL for process control, where an agent adjusts recipe parameters in real-time to maintain wafer uniformity [12]. The application of DRL to fault diagnosis is a burgeoning field. In this formulation, the diagnosis is treated as a game where the agent asks questions (queries sensors) or investigates components to isolate the fault with the minimum number of steps. This approach is particularly attractive because it balances exploration (gathering information about potential new fault types) and exploitation (quickly diagnosing known faults). However, applying DRL directly to raw sensor data can be unstable and computationally expensive. By constraining the DRL agent to operate within the structured environment of a Knowledge Graph, we can significantly reduce the search space and improve the semantic coherence of the agent's actions [13]. This intersection of graph-structured knowledge and reinforcement learning forms the basis of our proposed methodology.

3. Methodology

We propose a framework that integrates a domain-specific Knowledge Graph with a Deep Reinforcement Learning agent. The system operates in a continuous loop where sensor data triggers the diagnostic process, the agent navigates the graph to hypothesize a root cause, and the outcome updates both the graph statistics and the agent's policy.

3.1 Multi-Layer Knowledge Graph Construction

The foundation of our approach is a comprehensive Knowledge Graph (KG) that mirrors the cyber-physical reality of the wafer production line. We construct this graph using a multi-layer ontology. The first layer represents the Physical Entity Layer, comprising nodes for Tools, Chambers, Sensors, and Wafers. The second layer is the Process Layer, which includes nodes for Recipe Steps, Process Parameters (e.g., Temperature, Pressure, RF Power), and Time Intervals. The third layer is the Fault Layer, containing nodes for known Defect Classes, Failure Modes, and Root Causes. Edges in the graph represent specific relationships such as "has_sensor," "processed_by," "caused_by," or "correlated_with." To populate this graph, we ingest data from multiple sources including Equipment Interface logs, Manufacturing Execution Systems (MES), and Failure Analysis reports. We utilize Named Entity Recognition (NER) to extract entities from unstructured maintenance logs, linking them to structured sensor data. A crucial aspect of our KG construction is the inclusion of weighted edges representing the probability of causal links. For example, if historical data shows that a pressure deviation in Chamber A frequently leads to a particle defect, the edge connecting these nodes is assigned a high initial weight. These weights are dynamic and are updated as new production data becomes available, ensuring the graph reflects the current state of the machinery [14]. To facilitate the input for the neural network, we employ Graph Embedding techniques. Specifically, we use a graph neural network architecture to project the nodes and edges into a low-dimensional vector space while preserving their structural and semantic proximity. This embedding process transforms the symbolic graph into a numerical format suitable for processing by the DRL agent, allowing the system to understand that two tools sharing a common gas supply line are semantically close, even if they are spatially distant in the fab [15].

3.2 Graph-State Reinforcement Learning Agent

The core of our diagnostic engine is the Deep Reinforcement Learning agent. We formulate the fault diagnosis problem as a Markov Decision Process (MDP) over the Knowledge Graph. In this formulation, the environment is the weighted KG, and the agent is a virtual troubleshooter. The State space is defined by the current location of the agent on the graph and the sequence of nodes visited so far (the diagnostic path). Additionally, the state vector includes the current values of the sensor nodes connected to the agent's position. This allows the agent to perceive both the structural context and the real-time observational data. The Action space consists of moving to an adjacent node in the graph. For instance, if the agent is currently at a "Defect" node, it might choose to move to a "Process Step" node to investigate if a specific step was anomalous. Alternatively, it might move to a "Tool" node to check the equipment health. The set of valid actions is constrained by the graph topology, ensuring the agent follows logical links [16]. The Reward function is designed to encourage accuracy and efficiency. The agent receives a large positive reward for successfully identifying the correct root cause node (verified against labeled historical cases during training or operator feedback during deployment). Conversely, a small negative reward is applied for each step taken, incentivizing the agent to find the shortest path to the diagnosis. Significant negative rewards are assigned for incorrect diagnoses or for traversing into irrelevant sections of the graph. We utilize a Deep Q-Network (DQN) with a specialized architecture to approximate the Q-values for each action. The network takes the graph embedding of the current node and the history vector as input and outputs the expected utility of moving to each neighbor. To handle the variable number of neighbors (graph degree), we employ an attention mechanism that weighs the importance of adjacent nodes based on their edge attributes and the current diagnostic context [17]. This allows the agent to prioritize high-probability paths while still maintaining a non-zero probability of exploring less likely connections, which is essential for discovering novel fault mechanisms.

3.3 Adaptive Mechanism and Continuous Learning

A static diagnostic model inevitably degrades in a wafer fab due to concept drift. Tools degrade, chambers are cleaned, parts are replaced, and recipes are tuned. Our framework addresses this through a dual-adaptation strategy involving Graph Evolution and Policy Updates. Graph Evolution occurs when new entities or relations are detected. If a new sensor is installed, a node is added to the KG. If a new type of defect appears, it is initially added as an unknown node. As the system gathers data, statistical correlation analysis runs in the background to establish edges between this new defect and existing process parameters. This dynamic structural update ensures the environment represents the latest fab configuration [18]. Policy Updates ensure the DRL agent adapts to these structural changes. Unlike supervised models that require full retraining, DRL agents can employ experience replay with a bias toward recent experiences. When the graph changes, the agent explores the new regions (driven by an exploration bonus in the reward function). If the agent successfully diagnoses a fault using a new path involving the updated graph structure, this trajectory is stored in the replay buffer. Through continuous training iterations, the agent's policy shifts to incorporate the new knowledge. For example, if a recipe change makes "Temperature" a less reliable predictor of "Etch Rate" than "Gas Flow," the agent will learn to prioritize the path toward the "Gas Flow" node over time [19]. This adaptability allows the system to maintain high diagnostic performance even during ramp-up phases or process migrations.

4. Implementation and Experimental Design

To validate the proposed framework, we designed a rigorous set of experiments simulating a realistic semiconductor manufacturing environment. The implementation details and experimental setup are described below to ensure reproducibility and clarity regarding the evaluation metrics.

4.1 Data Description and Preprocessing

We utilized a hybrid dataset combining the publicly available SECOM dataset with a synthetic dataset generated from a proprietary wafer fab simulator. The SECOM dataset contains data from a semi-conductor manufacturing process with 591 features (sensor readings) and binary labels (pass/fail). To introduce the complexity required for graph-based analysis, we enriched this data using the simulator to generate topology information, effectively creating a "digital twin" metadata layer that maps the anonymous SECOM features to hypothetical tools, chambers, and process steps. The synthetic data generation involved simulating a production line with five major process steps: Cleaning, Deposition, Lithography, Etching, and Ion Implantation. We injected specific fault scenarios, such as "Mass Flow Controller drift in Etch Chamber 2" or "Focus offset in Lithography Scanner A." The combined dataset comprises approximately 100,000 wafer runs. Preprocessing involved normalizing sensor values using z-score standardization and discretizing continuous variables into state bins to facilitate the initial graph mapping. The resulting Knowledge Graph contained over 5,000 nodes and 25,000 relations. We partitioned the data chronologically to simulate the temporal nature of production, using the first 70% for initial training, 15% for validation, and the final 15% for testing adaptive performance [20].

4.2 Environment Configuration

The reinforcement learning environment was built using a standard OpenAI Gym interface wrapping the graph traversal logic. The state representation utilized a Graph Convolutional Network (GCN) to generate 64-dimensional embeddings for each node. The DRL agent was implemented using a Double DQN architecture to mitigate the overestimation bias of Q-values. The replay buffer size was set to 10,000 transitions, and we used an epsilon-greedy exploration strategy, decaying epsilon from 1.0 to 0.05 over the first 10,000 episodes.

We compared our proposed KG-DRL method against three baselines:

Random Forest (RF): A strong baseline for tabular data classification, trained on the flattened sensor vectors.

CNN-LSTM*:* A deep learning model combining convolutional layers for feature extraction and LSTM layers for temporal sequence analysis, representing the current state-of-the-art in pure data-driven diagnosis [21].

Static KG-Rule: A traditional knowledge graph approach using fixed rules and shortest-path algorithms without learning capabilities.

Table 1: Experimental Results comparing diagnostic accuracy and adaptability across different methods.

Method	Diagnostic Accuracy (%)	Convergence Time (Episodes/Epochs)	Adaptability Score (0-1)	Explainability
Random Forest	88.4	N/A (Batch)	0.35	Low (Feature Importance)
CNN-LSTM [21]	92.1	50 Epochs	0.42	Very Low (Black Box)
Static KG-Rule	76.5	N/A (Design)	0.15	High (Logic Trace)
Proposed KG-DRL	94.8	350 Episodes	0.89	High (Graph Path)

The "Adaptability Score" measures the drop in accuracy when a new fault type is introduced, with a higher score indicating less performance degradation. The experimental hardware consisted of a server with dual NVIDIA Tesla V100 GPUs and 256GB of RAM [22].

5. Results and Discussion

The evaluation focuses on three key dimensions: overall diagnostic accuracy, the ability to adapt to new fault conditions (concept drift), and the interpretability of the results.

5.1 Diagnostic Accuracy Analysis

As presented in Table 1, the proposed KG-DRL framework achieved the highest diagnostic accuracy at 94.8%. The Random Forest model performed adequately on known fault types but struggled to differentiate between complex, multi-variate failure modes that require understanding the sequence of operations. The CNN-LSTM model showed strong performance (92.1%), confirming the power of deep learning in pattern recognition. However, its slightly lower performance compared to KG-DRL can be attributed to its inability to explicitly leverage the topological dependencies between tools. For instance, if a defect in the "Etching" step is actually caused by a residue left during the preceding "Deposition" step, the CNN-LSTM might miss the correlation if the temporal lag is significant or variable. The KG-DRL agent, however, can traverse the "processed_after" link in the graph to investigate the upstream tool, effectively bridging the temporal gap through semantic connection [23]. The Static KG-Rule approach had the lowest accuracy. This highlights the limitation of relying solely on predefined expert rules. In a complex fab, the interactions are often too subtle or counter-intuitive for manual rule encoding. The DRL agent effectively "learns" the rules that are too complex to be explicitly programmed, identifying probabilistic paths that maximize diagnostic success.

5.2 Adaptability to Concept Drift

A critical component of our experiment was evaluating performance under changing conditions. At the 85% mark of the data stream, we introduced a simulated "recipe change" which altered the baseline values of several sensors and introduced a new failure mode related to a heater subsystem.

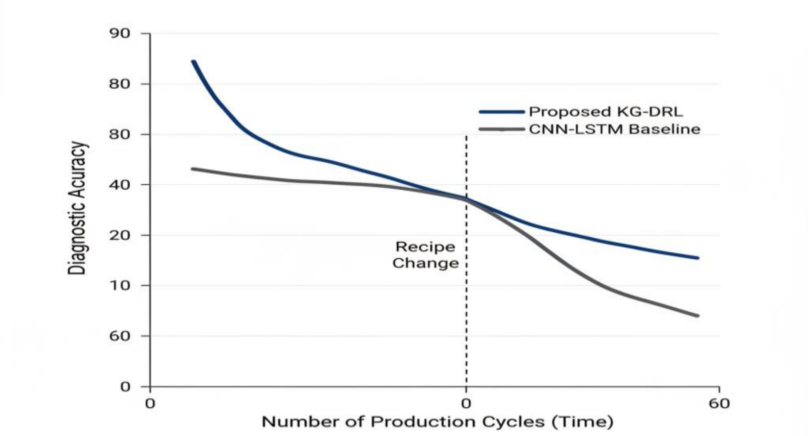

Figure 1: *Performance adaptation curves showing accuracy over time. The X*

Figure 1 illustrates the response of the models to this event. The CNN-LSTM model (and the Random Forest, not shown for clarity) suffered a significant drop in accuracy, falling below 60%. Recovering its performance required collecting a substantial amount of new labeled data and a full retraining cycle, represented by the slow upward slope. In contrast, the KG-DRL agent exhibited a much shallower dip. Because the graph was updated with the new sensor nodes and parameters, the agent could explore these new nodes. The exploration mechanism inherent in Reinforcement Learning allowed the agent to test new hypotheses rapidly. Within a short number of episodes, the agent adjusted its policy to incorporate the new sensor readings, returning to near-peak accuracy significantly faster than the supervised baselines. This result validates the hypothesis that fusing DRL with KGs provides superior resilience to the dynamic nature of wafer production [24].

5.3 Interpretability and Operational Trust

Beyond raw metrics, the operational value of the system depends on user trust. The "Explainability" column in Table 1 summarizes the qualitative assessment. When the CNN-LSTM predicts a fault, it provides a probability score but no context. Engineers must still dig through logs to understand "why." In contrast, the output of our KG-DRL agent is a path through the graph: "Start -> Wafer_ID -> Etch_Chamber_B -> Pressure_Sensor_4 -> High_Variance -> Fault: Mass_Flow_Instability." This path serves as a narrative explanation. It tells the engineer exactly which components were investigated and in what order. We conducted a small user study with process engineers who reviewed the outputs of both systems. The feedback overwhelmingly favored the KG-DRL output, as it aligned with their standard root cause analysis workflows. This semantic transparency reduces the "Mean Time To Validate" a diagnosis, further enhancing the overall efficiency of the maintenance cycle [25].

6. Conclusion

This paper presented a novel framework for adaptive fault diagnosis in wafer production lines by fusing Knowledge Graphs with Deep Reinforcement Learning. By modeling the complex, heterogeneous data of a semiconductor fab into a semantic graph, we created an environment that reflects the physical and logical topology of the manufacturing process. The integration of a DRL agent allows for dynamic navigation of this graph, transforming diagnosis from a static classification task into an adaptive search process. Our experimental results demonstrate that this approach yields superior diagnostic accuracy compared to traditional machine learning and deep learning baselines. More importantly, the system exhibits remarkable resilience to concept drift, rapidly adapting to recipe changes and new equipment configurations that typically cripple supervised models. The inherent explainability of the graph traversal provides engineers with actionable insights, bridging the gap between AI capabilities and human operational requirements.

Future work will focus on scaling the system to handle multi-fab environments where knowledge can be transferred between different production lines (Transfer Learning). Additionally, we aim to incorporate Federated Learning techniques to allow the training of the graph embeddings across different organizations without sharing sensitive proprietary process data. As semiconductor manufacturing continues to advance in complexity, such adaptive, intelligible, and robust diagnostic systems will be instrumental in securing the yields of the future.

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