Overview of the Application of Artificial Intelligence in Semiconductor Manufacturing Process Optimization and Defect Detection

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Abstract Semiconductor manufacturing involves highly complex and tightly coupled process flows, stringent quality requirements, and the generation of vast amounts of heterogeneous data throughout the entire manufacturing lifecycle. As device dimensions shrink and process integration becomes increasingly complex, traditional statistical and physics-based methods face growing limitations in handling nonlinear interactions, process variability, and real-time decision-making needs. Therefore, artificial intelligence (AI) has emerged as an effective data-driven approach to enhance manufacturing performance by enabling advanced process modeling, optimization, and fault analysis. This paper reviews the latest advancements in the application of artificial intelligence in semiconductor manufacturing, with a particular focus on process optimization and defect detection. It explores the applications of AI in process parameter optimization, yield improvement, and virtual metrology, highlighting its role in reducing variability and improving manufacturing efficiency.

Keywords Semiconductor manufacturing, Process optimization, Defect detection, Fault diagnosis, Machine learning, Deep learning

1 Introduction

Semiconductor manufacturing is one of the most complex and capital-intensive industrial processes, involving hundreds of tightly coupled steps such as lithography, etching, deposition, ion implantation, and chemical mechanical planarization. As device dimensions continue to scale down and process integration becomes increasingly sophisticated, semiconductor fabrication systems generate massive volumes of high-dimensional, heterogeneous, and time-dependent data (Moyne & Tilbury, 2007). Managing process variability, improving yield, and ensuring stable production performance have therefore become central challenges for modern semiconductor fabs.

Traditionally, process monitoring and control in semiconductor manufacturing have relied on statistical process control (SPC), fault detection and classification (FDC), and physics-based process models (Montgomery, 2009). While these methods have proven effective under relatively stable and well-understood conditions, their performance degrades in advanced manufacturing nodes characterized by nonlinear process interactions, tool-to-tool variations, and limited measurement accessibility (Good & Qin, 2011). In addition, many critical process parameters cannot be measured in real time due to cost, throughput, or physical constraints, further limiting the effectiveness of conventional approaches (Kang et al., 2018).

In recent years, artificial intelligence (AI) and machine learning (ML) techniques have emerged as promising solutions to address these challenges. By learning complex relationships directly from large-scale manufacturing data, AI-based methods offer enhanced capabilities for modeling nonlinear processes, handling high-dimensional inputs, and adapting to dynamic production environments (Jordan & Mitchell, 2015). As a result, AI has been increasingly applied across various stages of semiconductor manufacturing, particularly in process optimization and defect detection tasks (Lee et al., 2021).

Process optimization is a critical objective in semicon-

ISSN 3106-7018 (Print) ISSN 3106-5791 (Online)

ductor manufacturing, as small improvements in process parameters can lead to substantial gains in yield and cost efficiency. Machine learning models have been widely used to predict key process outcomes, optimize operating conditions, and reduce process variability (Qin, 2014). Applications such as virtual metrology enable the estimation of unmeasured quality variables using sensor and equipment data, thereby reducing reliance on expensive or time-consuming physical measurements (Kang et al., 2018). More recently, deep learning and reinforcement learning approaches have been explored for adaptive process control, enabling dynamic parameter tuning in response to changing process conditions (Zhang et al., 2020).

Defect detection and fault diagnosis represent another major application domain of AI in semiconductor manufacturing. Wafer defects, equipment malfunctions, and process abnormalities can significantly degrade product quality and production yield if not detected at an early stage (Jin et al., 2001). Traditional rule-based and statistical methods often struggle to capture subtle defect patterns or complex fault signatures, especially in advanced technology nodes (Tsai & Chen, 2017). In contrast, AI-based approaches—particularly convolutional neural networks—have demonstrated strong performance in wafer map analysis, defect classification, and image-based inspection tasks (Nakazawa et al., 2019). Furthermore, data-driven fault diagnosis and predictive maintenance systems have been shown to reduce unplanned downtime and improve equipment reliability in semiconductor fabs (Lee et al., 2020).

Despite the growing body of research, the application of AI in semiconductor manufacturing still faces several challenges. Data quality and availability remain significant obstacles, as labeled defect data are often scarce and manufacturing data are subject to noise and distribution shifts (Yoon et al., 2021). In addition, the lack of model interpretability raises concerns regarding trust, accountability, and integration with existing manufacturing decision systems (Rudin, 2019). These issues highlight the need for systematic reviews that can synthesize existing research findings, identify practical limitations, and plan future research directions. This paper provides an overview of the application of artificial intelligence in semiconductor manufacturing, with a specific focus on process optimization and defect detection.

2 Artificial Intelligence Methods Used in Semiconductor Manufacturing

The application of artificial intelligence in semiconductor manufacturing primarily relies on data-driven modeling techniques that can capture complex, nonlinear relationships between process variables and manufacturing outcomes. Depending on the nature of the data and the target task, AI methods used in semiconductor fabs can be broadly categorized into traditional machine learning approaches, deep learning models, and reinforcement learning–based techniques (Qin, 2014; Yoon et al., 2021).

2.1 Traditional Machine Learning Methods

Traditional machine learning methods remain widely used in semiconductor manufacturing due to their relatively low computational cost, robustness with limited data, and interpretability. Techniques such as support vector machines (SVM), decision trees, random forests, k-nearest neighbors (kNN), and linear or nonlinear regression models have been extensively applied to process modeling, fault detection, and yield prediction tasks (Jin et al., 2001; Tsai & Chen, 2017).

Dimensionality reduction and feature extraction techniques, including principal component analysis (PCA) and independent component analysis (ICA), are often employed as preprocessing steps to address the high dimensionality and multicollinearity commonly observed in semiconductor process data (Good & Qin, 2011). These methods are particularly effective in statistical process monitoring and fault detection applications, where deviations from normal operating conditions must be identified in a reliable and interpretable manner (Montgomery, 2009). Despite their advantages, traditional machine learning approaches generally require careful feature engineering and may struggle to model highly nonlinear or time-dependent processes encountered in advanced semiconductor manufacturing nodes (Qin, 2014).

2.2 Deep Learning Approaches

With the increasing availability of large-scale manufacturing data and advances in computing hardware, deep learning techniques have gained significant attention in semiconductor manufacturing applications. Deep neural networks are capable of automatically learning hierarchical feature representations from raw data, making them well suited for complex and high-dimensional problems (LeCun et al., 2015).

Convolutional neural networks (CNNs) have been widely adopted for image-based tasks such as wafer map analysis, defect pattern recognition, and optical inspection, where spatial correlations play a critical role (Nakazawa et al., 2019). Recurrent neural networks (RNNs), including long short-term memory (LSTM) architectures, are commonly used to model time-series sensor data for process monitoring and equipment health assessment (Zhang et al., 2020). Autoencoder-based models have also been applied for unsupervised anomaly detection and feature learning in situations where labeled defect data are scarce (Sakurada & Yairi, 2014). Although deep learning methods often achieve superior predictive performance, their deployment in semiconductor manufacturing is challenged by issues related to data labeling costs, model interpretability, and robustness under changing process conditions (Rudin, 2019; Yoon et al., 2021).

2.3 Reinforcement Learning and Hybrid Approaches

Reinforcement learning (RL) has emerged as a promising approach for adaptive process optimization in semiconductor manufacturing. Unlike supervised learning methods, RL focuses on learning optimal control policies through interactions with the environment, making it suitable for sequential decision-making problems such as dynamic process parameter tuning (Sutton & Barto, 2018).

In recent studies, RL has been applied to tasks including recipe optimization, equipment scheduling, and adaptive control of manufacturing processes (Zhang et al., 2020). To address data efficiency and safety concerns, hybrid approaches that combine reinforcement learning with physics-based models or simulation environments have been proposed (Lee et al., 2015). These hybrid methods aim to leverage domain knowledge while retaining the adaptability of AI-based techniques. Overall, the selection of AI methods in semiconductor manufacturing is highly task-dependent and influenced by factors such as data availability, system complexity, and real-time requirements. In practice, hybrid frameworks that integrate multiple AI techniques are increasingly adopted to balance performance, interpretability, and deployment feasibility (Qin, 2014; Yoon et al., 2021).

3 AI for Process Optimization in Semiconductor Manufacturing

Process optimization is a critical objective in semiconductor manufacturing, as minor deviations in process parameters can lead to significant variations in device performance, yield, and production cost. The increasing complexity of advanced manufacturing nodes has made it difficult for traditional rule-based or physics-driven approaches to fully capture the nonlinear interactions among process variables (Qin, 2014). As a result, AI-based methods have been widely adopted to enhance process modeling accuracy, optimize operating conditions, and reduce process variability.

3.1 Process Parameter Modeling and Optimization

AI techniques have been extensively used to model the relationships between process parameters and key quality indicators in semiconductor manufacturing. Supervised machine learning models, such as support vector machines and random forests, are commonly employed to predict process outcomes including critical dimension (CD), film thickness, and electrical performance metrics based on sensor and equipment data (Jin et al., 2001; Lee et al., 2021). With the advancement of deep learning, neural network–based models have demonstrated improved capability in capturing highly nonlinear process behaviors. These models enable more accurate prediction of process responses under varying operating conditions, supporting data-driven optimization of parameters such as exposure dose, etching time, and deposition rates (LeCun et al., 2015; Zhang et al., 2020). In practice, AI-based optimization frameworks are often integrated with existing process control systems to recommend optimal parameter settings rather than directly replacing human decision-making (Qin, 2014).

3.2 Yield Enhancement and Variability Reduction

Yield improvement is a central concern in semiconductor fabs, particularly for advanced technology nodes where defect tolerance is minimal. AI-based predictive models have been widely applied to estimate yield loss contributors and identify critical process steps that dominate yield variability (Lee et al., 2021). By analyzing historical manufacturing data, machine learning models can uncover hidden correlations between process variables

ISSN 3106-7018 (Print) ISSN 3106-5791 (Online)

and yield outcomes that are difficult to identify using conventional statistical methods (Good & Qin, 2011). In addition to yield prediction, AI techniques have been used to reduce process variability by enabling more consistent control across tools, chambers, and production lots. For example, data-driven models can compensate for tool-to-tool differences by adjusting control parameters based on equipment-specific behavior, thereby improving overall process uniformity (Yoon et al., 2021). These approaches are particularly valuable in high-mix manufacturing environments where frequent recipe changes are required.

3.3 Virtual Metrology and Predictive Process Control

Virtual metrology (VM) is one of the most successful AI-driven applications in semiconductor process optimization. VM aims to estimate quality variables that are difficult or costly to measure in real time by using readily available process and sensor data (Kang et al., 2018). Machine learning models, including regression-based methods and neural networks, have been widely adopted for VM applications across lithography, etching, and deposition processes. By providing real-time estimates of process quality, VM enables predictive process control and early detection of abnormal trends before physical measurements become available (Kang et al., 2018). This capability allows manufacturers to take corrective actions earlier in the production cycle, reducing scrap rates and improving throughput. Recent studies have also explored combining VM with adaptive learning techniques to maintain model accuracy under process drift and changing manufacturing conditions (Zhang et al., 2020).

3.4 Reinforcement Learning for Adaptive Process Optimization

Reinforcement learning has gained increasing attention as a tool for adaptive process optimization in semiconductor manufacturing. Unlike static predictive models, reinforcement learning focuses on sequential decision-making and policy optimization, making it suitable for dynamic control scenarios where process conditions evolve over time (Sutton & Barto, 2018). In semiconductor applications, reinforcement learning has been explored for optimizing process recipes, adjusting control parameters, and managing trade-offs between yield, throughput, and equipment utilization (Zhang et al., 2020). To mitigate risks associated with direct online learning, reinforcement learning is often implemented in conjunction with simulation environments or digital twins, allowing policies to be trained and validated before deployment in real manufacturing systems (Lee et al., 2015). Overall, AI-based process optimization techniques have demonstrated significant potential to improve manufacturing efficiency, yield stability, and operational flexibility. However, their successful deployment requires careful consideration of data quality, model robustness, and integration with existing manufacturing execution and control systems (Yoon et al., 2021).

4 AI for Defect Detection and Fault Diagnosis in Semiconductor Manufacturing

Defect detection and fault diagnosis are essential components of quality assurance and reliability management in semiconductor manufacturing. Defects originating from process deviations, equipment malfunctions, or material inconsistencies can significantly impact device performance and yield if not identified in a timely manner (Jin et al., 2001). As manufacturing processes become more complex and data-intensive, traditional inspection and monitoring methods face increasing limitations, motivating the adoption of AI-based approaches for more accurate and scalable defect analysis.

4.1 Wafer Defect Detection and Classification

Wafer-level defects are among the most critical quality issues in semiconductor manufacturing, as they directly affect device functionality and yield. Conventional defect inspection methods rely on rule-based image processing and statistical analysis, which often struggle to capture complex and subtle defect patterns in advanced technology nodes (Tsai & Chen, 2017). AI-based methods, particularly deep learning techniques, have demonstrated strong performance in wafer defect detection and classification tasks.

Convolutional neural networks (CNNs) are widely used for analyzing wafer map patterns and inspection images due to their ability to extract spatial features automatically (Nakazawa et al., 2019). These models can classify defect types such as scratches, particles, and systematic pattern defects with higher accuracy than traditional approaches. In addition, unsupervised and semi-supervised learning methods have been explored to address the limited availability of labeled defect data, enabling anomaly detection without extensive manual annotation (Sakurada & Yairi, 2014).

4.2 Equipment Fault Detection and Diagnosis

Equipment-related faults are a major source of yield loss and unplanned downtime in semiconductor fabs. Modern manufacturing tools are equipped with numerous sensors that generate large volumes of time-series data, providing opportunities for data-driven fault detection and diagnosis (Moyne & Tilbury, 2007). AI-based models have been widely applied to identify abnormal equipment behavior and diagnose underlying fault causes.

Traditional machine learning methods, including support vector machines and decision trees, have been used for equipment fault classification based on sensor features and process indicators (Jin et al., 2001). More recently, deep learning models such as recurrent neural networks and long short-term memory networks have been employed to capture temporal dependencies in sensor data, improving fault detection accuracy for complex equipment dynamics (Zhang et al., 2020). These approaches enable earlier detection of equipment degradation and support proactive maintenance strategies.

4.3 Predictive Maintenance and Early Fault Warning

Predictive maintenance aims to anticipate equipment failures before they occur, thereby reducing unplanned downtime and maintenance costs. AI-based predictive maintenance systems leverage historical and real-time data to estimate equipment health and remaining useful life (Lee et al., 2020). By identifying early warning signals associated with impending failures, these systems enable timely maintenance interventions and improve overall equipment effectiveness.

In semiconductor manufacturing, predictive maintenance applications often integrate anomaly detection models with fault diagnosis frameworks to provide comprehensive equipment health monitoring (Yoon et al., 2021). Unsupervised learning methods, such as autoencoders and clustering techniques, are particularly valuable for detecting previously unseen fault modes. However, challenges remain in ensuring model robustness under changing process conditions and integrating predictive maintenance outputs into existing manufacturing execution systems.

4.4 Challenges in AI-Based Defect Detection and Diagnosis

Despite their demonstrated effectiveness, AI-based defect detection and fault diagnosis methods face several practical challenges. One major issue is the scarcity of labeled defect and fault data, as many failure events occur infrequently and are costly to reproduce (Tsai & Chen, 2017). In addition, variations in equipment configuration, process recipes, and production environments can limit the generalization ability of trained models (Yoon et al., 2021).

Model interpretability is another critical concern, particularly in high-stakes manufacturing environments where engineers must understand and trust AI-driven decisions (Rudin, 2019). As a result, there is growing interest in combining AI models with domain knowledge and explainable AI techniques to enhance transparency and adoption in semiconductor fabs. Overall, AI-based defect detection and fault diagnosis technologies have become indispensable tools for improving manufacturing quality and reliability. Continued research is needed to address data limitations, enhance model robustness, and facilitate seamless integration with industrial manufacturing systems.

5 Challenges and Future Trends

Despite the rapid progress and demonstrated benefits of artificial intelligence in semiconductor manufacturing, several challenges continue to limit its large-scale deployment and long-term effectiveness. Addressing these issues is essential for transitioning AI-based methods from experimental tools to reliable components of production-grade manufacturing systems.

5.1 Data Quality, Availability, and Labeling

One of the most significant challenges in applying AI to semiconductor manufacturing is data-related. Manufacturing data are often noisy, incomplete, and heterogeneous, originating from multiple tools, sensors, and process steps (Moyne & Tilbury, 2007). In addition, labeled data for defects and equipment faults are typically scarce, as failure events occur infrequently and labeling requires substantial domain expertise (Tsai & Chen, 2017).

These limitations reduce the effectiveness of supervised learning methods and motivate the development of unsu-

ISSN 3106-7018 (Print) ISSN 3106-5791 (Online)

pervised, semi-supervised, and weakly supervised learning approaches (Sakurada & Yairi, 2014). Future research is expected to focus on data-efficient learning strategies, including transfer learning and few-shot learning, to improve model performance under limited labeled data conditions (Yoon et al., 2021).

5.2 Model Robustness and Generalization

Another critical challenge is the robustness and generalization of AI models under changing manufacturing conditions. Process drift, equipment aging, and recipe updates can cause significant distribution shifts between training and deployment data, leading to degraded model performance over time (Qin, 2014). Ensuring that AI models remain accurate and reliable in dynamic production environments remains an open problem.

Adaptive learning, online model updating, and domain adaptation techniques are increasingly being explored to address these issues (Zhang et al., 2020). However, implementing such methods in real manufacturing systems requires careful consideration of stability, safety, and computational constraints.

5.3 Interpretability and Trustworthiness

The lack of interpretability in many AI models, particularly deep learning approaches, poses a major barrier to adoption in semiconductor manufacturing. Engineers and decision-makers must be able to understand and trust AI-driven recommendations, especially in high-stakes production environments where incorrect decisions can lead to substantial financial losses (Rudin, 2019).

As a result, explainable AI (XAI) techniques and hybrid modeling approaches that combine data-driven models with physical insights are gaining increasing attention (Rudin, 2019; Qin, 2014). Physics-informed machine learning methods, which embed domain knowledge and physical constraints into learning algorithms, represent a promising direction for improving model transparency and reliability (Karniadakis et al., 2021).

5.4 Integration with Manufacturing Systems and Digital Twins

Seamless integration of AI models with existing manufacturing execution systems (MES), process control frameworks, and decision-support tools remains a practical challenge. AI solutions must operate within strict real-time, safety, and reliability requirements, which are not always considered in academic studies (Lee et al., 2015).

Looking forward, digital twin technology is expected to play a central role in enabling more effective AI-driven optimization and fault diagnosis. By combining high-fidelity simulations with real-time manufacturing data, digital twins provide a controlled environment for training, validating, and deploying AI models with reduced operational risk (Tao et al., 2019). The integration of AI, digital twins, and closed-loop control systems represents a key future trend in semiconductor manufacturing.

5.5 Future Research Directions

Future research on AI in semiconductor manufacturing is likely to focus on several interconnected directions. These include the development of data-efficient and robust learning algorithms, greater emphasis on model interpretability and trustworthiness, and tighter integration of AI with physical models and manufacturing systems (Yoon et al., 2021). In addition, as advanced technology nodes such as EUV lithography and gate-all-around transistors become more prevalent, AI methods will need to adapt to increasingly complex and data-intensive process environments.

Overall, overcoming current challenges and leveraging emerging technologies will be critical for realizing the full potential of artificial intelligence as a core enabler of next-generation semiconductor manufacturing.

6 Conclusion

Artificial intelligence has become an increasingly important enabler for improving efficiency, yield, and reliability in semiconductor manufacturing. As reviewed in this paper, AI-based approaches have demonstrated significant advantages over traditional statistical and physics-based methods in handling high-dimensional, nonlinear, and data-intensive manufacturing environments (Qin, 2014; Yoon et al., 2021). By leveraging large volumes of process, equipment, and inspection data, AI techniques provide new opportunities for data-driven decision-making across the semiconductor manufacturing lifecycle.

In the context of process optimization, machine learning and deep learning models have been widely applied to process parameter modeling, yield enhancement, and virtual metrology. These approaches enable more accurate prediction of process outcomes and support proactive control strategies, contributing to reduced variability and improved manufacturing consistency (Kang et al., 2018; Lee et al., 2021). Reinforcement learning and adaptive optimization frameworks further extend these capabilities by addressing dynamic and sequential decision-making problems in complex process environments (Zhang et al., 2020).

For defect detection and fault diagnosis, AI-based methods—particularly deep learning models—have shown strong performance in wafer defect classification, equipment fault detection, and predictive maintenance. Compared with traditional rule-based and statistical techniques, AI-driven approaches offer enhanced sensitivity to subtle defect patterns and early fault signatures, enabling faster response and reduced production losses (Nakazawa et al., 2019; Lee et al., 2020). These capabilities are increasingly critical as semiconductor manufacturing advances toward smaller technology nodes and higher integration densities.

Despite these advances, several challenges remain before AI can be fully integrated as a core component of semiconductor manufacturing systems. Issues related to data quality, model robustness, interpretability, and system integration continue to limit large-scale deployment in production environments (Rudin, 2019; Yoon et al., 2021). Addressing these challenges will require closer integration of AI models with domain knowledge, physical principles, and manufacturing infrastructure.

Looking forward, future research is expected to focus on data-efficient learning, explainable and physics-informed AI, and tighter coupling between AI, digital twins, and closed-loop process control systems (Karniadakis et al., 2021; Tao et al., 2019). As these technologies mature, artificial intelligence is poised to evolve from an auxiliary analytical tool into a central decision-making element in next-generation semiconductor manufacturing. Continued interdisciplinary collaboration between AI researchers, process engineers, and manufacturing practitioners will be essential to fully realize this potential.

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