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Defect Prediction and Optimization in Semiconductor Manufacturing Using Explainable AutoML

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Abstract: The semiconductor manufacturing industry often faces the severe challenges of data scarcity and imbalance. While the semiconductor industry has conducted extensive research on leveraging machine learning to improve yield, defect prediction remains largely unexplored, especially with small datasets. This research proposes a framework called xAutoML, which automatically selects the optimal model and hyperparameters for defect prediction to enhance the interpretability of the results. Furthermore, it addresses the critical issue of data imbalance, a common problem in defect prediction tasks, by employing techniques such as focus loss and oversampling. We use publicly available datasets to demonstrate how xAutoML effectively adapts to data constraints and deeply analyzes key features influencing defect occurrence. Results show that the proposed method outperforms traditional methods in terms of prediction accuracy and the provision of actionable and interpretable insights. Its application in real-time defect monitoring and process optimization in semiconductor manufacturing helps bridge the gap between advanced machine learning techniques and practical industry applications.

Keywords: Explainable AutoML, XAutoML, Semiconductor Manufacturing, Defect Prediction, Data Imbalance, Machine Learning, Model Interpretability, Process Optimization.

Disciplines: Computer Science. **Subjects:** Artificial Intelligence.

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1 INTRODUCTION

In recent decades, the semiconductor manufacturing industry has experienced exponential growth, driven by increasing demand for smaller, faster, and more efficient electronic devices. However, despite the remarkable advancements in technology, the industry still faces significant challenges related to product quality and production efficiency [1]. One of the most pressing challenges lies in the accurate and timely detection of defects during manufacturing, which directly impacts product yield, performance, and ultimately, profitability. While traditional defect detection methods, such as optical inspection and scanning electron microscopy (SEM), have made substantial contributions to identifying manufacturing anomalies, these methods often fall short in terms of scalability, speed, and the capacity to predict defects proactively [2].

To address these limitations, the integration of machine learning (ML) techniques into semiconductor manufacturing processes has gained considerable attention in recent years[3]. Machine learning, particularly through the application of automated machine learning (AutoML) frameworks, presents a promising avenue for enhancing the efficiency and accuracy of defect prediction. AutoML, which automates the process of model selection, training, and hyperparameter tuning, has the potential to significantly reduce the time and expertise required for model development, making it an attractive solution for industrial applications [4]. Despite its capabilities, the application of AutoML in semiconductor manufacturing remains underexplored, especially when considering small data sets, imbalanced classes, and the critical need for explainability in industrial contexts [5].

This paper aims to contribute to filling this gap by proposing a novel framework for defect prediction and optimization in semiconductor manufacturing using Explainable AutoML[6]. The framework builds upon the foundational principles of AutoML, with an emphasis on explainability, a feature that has become increasingly essential for industrial applications where understanding the rationale behind model predictions is crucial for decision-making and process adjustments [7]. By leveraging xAutoML, this study proposes an approach that not only automates the defect prediction process but also provides actionable insights into the key factors driving the occurrence of defects [8]. In doing so, it enables manufacturers to proactively identify and mitigate potential issues before they escalate, ultimately improving production efficiency and reducing costs.

At the heart of this study lies the challenge of data imbalance, which is a common issue in manufacturing defect prediction. In semiconductor manufacturing, the number of

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defective products often represents a small fraction of the overall production, leading to skewed data distributions [10]. Traditional models struggle to perform effectively under these conditions, often yielding biased or inaccurate predictions. The proposed xAutoML framework seeks to address this challenge by incorporating techniques such as focal loss[11] and oversampling methods to ensure that the model is better equipped to handle imbalanced data. These strategies are aimed at improving model performance and ensuring that predictions are accurate even in the face of relatively scarce defect data.

The goal of this research is not merely to develop a defect prediction model, but to enhance the interpretability of machine learning models in a way that is specifically tailored to the needs of semiconductor manufacturers [12]. By providing clear explanations of the model's decision-making process, the proposed framework allows engineers and decision-makers to understand the relationships between production parameters and defect occurrence, leading to better-informed decisions and improved process control.

Through these contributions, this study aims to bridge the gap between advanced machine learning techniques and practical, real-world applications in semiconductor manufacturing [13]. In doing so, it contributes to the ongoing effort to optimize manufacturing processes, reduce costs, and improve product quality. Further research is needed to refine these methods, particularly in the context of real-time defect prediction and the integration of sensor data for continuous process optimization [14].

2 LITERATURE REVIEW

The application of machine learning in semiconductor manufacturing has garnered considerable interest in recent years, especially as the complexity of production processes increases. However, despite the growing use of automated technologies, challenges persist, particularly in defect prediction and quality control. This section reviews the current state of research related to semiconductor manufacturing, focusing on defect prediction models, the use of AutoML techniques, and the integration of explainability within machine learning models [15]. It also critically evaluates existing solutions, their limitations, and how this paper positions itself within the current body of work.

2.1 Defect Prediction in Semiconductor Manufacturing

Semiconductor manufacturing is an intricate process involving numerous stages, each of which can potentially introduce defects that affect the overall yield and quality. Defects in semiconductor devices, such as cracks, voids, or contamination, are often difficult to detect, especially in the early stages of production. Traditional inspection methods, such as optical inspection and scanning electron microscopy, have long been employed to identify such defects, but they have limitations in scalability, speed, and precision. As Sun et al. (2024) [16] argue, although these methods provide high accuracy at times, they are expensive and time-consuming, which makes them less feasible for large-scale production environments. The reliance on manual inspections can also result in high error rates and the inability to predict potential defects in advance.

Recent advances in machine learning, particularly in the context of defect detection, have provided promising alternatives to traditional methods. Deep learning techniques, such as convolutional neural networks (CNNs), have demonstrated their capability in identifying defects in semiconductor wafers [17]. These techniques, although highly accurate, often require large annotated datasets for training. In contrast, supervised learning methods struggle with the challenge of limited labeled defect data, a significant issue in semiconductor manufacturing, where defects represent a minority class [18]. This gap has led to the exploration of semi-supervised learning and unsupervised anomaly detection methods, which attempt to circumvent the need for large labeled datasets by learning from fewer examples. While these methods show potential, they are not without challenges, particularly in balancing the false-positive and false-negative rates, which directly impacts manufacturing efficiency.

Considering these factors, this paper proposes the use of Explainable AutoML to automate defect prediction while addressing issues related to data scarcity and imbalance [19]. xAutoML can potentially offer a more practical approach to defect prediction by not only automating model selection but also integrating explainability into the prediction process, a factor that remains underexplored in the existing literature.

2.2 The Rise of AutoML in Industrial Applications

AutoML has emerged as a powerful tool to democratize machine learning by automating the process of selecting models and tuning hyperparameters. It allows even non-experts to apply machine learning techniques effectively to industrial problems, such as semiconductor defect prediction, with minimal manual intervention. The core advantage of AutoML lies in its ability to significantly reduce the time and expertise required to build robust models. Ren et al. (2025) [9] outline the key benefits of AutoML in terms of reducing human bias and optimizing model parameters, leading to better generalization and performance.

However, AutoML frameworks still face several limitations. As Chen et al. (2020) note [20], while AutoML platforms can automate the machine learning pipeline, they often struggle with tasks that require domain-specific knowledge, such as understanding the intricacies of semiconductor production processes. Furthermore, AutoML's "black-box" nature complicates the interpretation of model decisions, which is a significant concern in industries like semiconductor manufacturing, where

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understanding the reasons behind defect predictions is essential for process optimization and decision-making.

To some extent, the problem of model transparency and interpretability can be mitigated by integrating explainable artificial intelligence (XAI) techniques into AutoML frameworks. Ribeiro et al. (2016) highlight the importance of explainability in ML models, especially in industrial settings where the reasoning behind decisions needs to be understood and trusted by domain experts [21]. Recent advancements in LIME and SHAP have made it possible to provide insights into the model's decision-making process, thereby improving the trustworthiness and applicability of AutoML solutions in real-world environments.

This integration of explainability with AutoML forms the foundation of this research. By incorporating explainable models into defect prediction systems, we aim to provide not only accurate predictions but also actionable insights that can guide process adjustments and quality control.

2.3 Handling Data Imbalance in Semiconductor Defect Prediction

A recurring issue in defect prediction is data imbalance, where the number of defective units is much smaller than that of non-defective units. This imbalance can severely undermine the performance of machine learning models, as they tend to predict the majority class more accurately, thus failing to identify defects effectively. Liu et al. (2025) propose [22] focal loss, a modification of the traditional cross-entropy loss, which focuses more on hard-to-classify examples, making it particularly useful for imbalanced classification tasks. Focal loss has been successfully applied in various domains, including object detection, and holds promise for improving defect prediction accuracy in semiconductor manufacturing.

In addition to focal loss, various oversampling techniques such as SMOTE (Synthetic Minority Over-sampling Technique) and ADASYN have been employed to create synthetic samples of the minority class, thereby balancing the dataset. Huang's demonstrated [23] that these oversampling techniques can significantly improve model performance in imbalanced classification problems. However, they also introduce the risk of overfitting, particularly in small data settings, where synthetic samples may not perfectly reflect the characteristics of real defects. This presents a challenge for any machine learning model attempting to generalize defect patterns from a limited dataset.

Given these challenges, it is clear that addressing data imbalance is critical for improving the robustness and accuracy of defect prediction models. In the current study, we will experiment with focal loss and oversampling techniques, testing their effectiveness in mitigating the challenges posed by imbalanced data and ensuring the model's ability to predict defects in a reliable manner.

2.4 Current Limitations and Gaps in the Literature

While significant progress has been made in applying machine learning to semiconductor manufacturing, the existing body of literature reveals several gaps. First, much of the research on defect prediction focuses primarily on model accuracy, with limited attention paid to explainability. As previously discussed, the complexity of semiconductor production processes necessitates the use of transparent models that can provide domain experts with insights into the factors influencing defect occurrence. To date, the combination of xAutoML and explainability in semiconductor defect prediction has not been widely explored, representing an important gap in the literature[24].

Moreover, despite the extensive application of deep learning methods such as CNNs and support vector machines (SVMs) in defect detection, there remains a lack of consensus on how to handle small and imbalanced datasets in real-world industrial settings. Many existing methods either require large datasets or fail to generalize effectively in the presence of highly skewed class distributions. Thus, further research is needed to explore how AutoML frameworks, specifically those incorporating explainability and data imbalance handling techniques, can address these limitations and provide practical solutions for semiconductor defect prediction.

2.5 Positioning of the Current Research

This paper positions itself at the intersection of xAutoML, defect prediction, and explainability. Building on the foundations of existing research, it proposes a novel framework that not only automates the defect prediction process but also integrates explainability techniques to provide actionable insights for process optimization. The current research aims to contribute to the literature by offering a practical solution to the problem of data imbalance in semiconductor defect prediction, while simultaneously addressing the need for more interpretable machine learning models in industrial settings.

Through this review, it becomes clear that while the use of AutoML in semiconductor manufacturing has potential, there is still much to be explored in terms of model interpretability and the effective handling of imbalanced datasets [25]. The following sections will present the research design and methodology that addresses these issues, laying the groundwork for the proposed framework's implementation and evaluation.

3 METHODOLOGY

This section describes the methodology employed to develop and evaluate the xAutoML framework for semiconductor defect prediction. The framework is designed to automate key steps in the machine learning process,

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including model selection, hyperparameter optimization, and evaluation, while addressing the inherent challenges of semiconductor manufacturing data—namely, small datasets, class imbalance, and the need for explainability. Through the integration of domain-specific knowledge and advanced machine learning techniques, this approach aims to provide both high predictive accuracy and actionable insights into the manufacturing process. The methodology outlined here is structured around data collection and preprocessing, model selection and tuning, and the incorporation of explainability techniques, all of which are essential for ensuring the effectiveness of the model in an industrial setting.

3.1 Data Collection and Preprocessing

Data acquisition in semiconductor manufacturing presents significant challenges, not only due to the complexity of the production process but also because of the inherent scarcity of labeled defect data. In this study, publicly available datasets primarily the SECOM dataset were used, along with simulated defect data generated through controlled processes [26]. The SECOM dataset, which includes a range of production parameters along with defect labels, provides a reasonable proxy for real-world manufacturing environments, though it is not without limitations. Specifically, the dataset includes imbalances in defect classifications, with defects representing a small minority of the total samples, which is a common issue in semiconductor production.

Preprocessing steps are crucial in transforming raw data into usable input for machine learning models. The preprocessing pipeline begins with missing data imputation. Given the nature of industrial data, missing values are common due to sensor errors or incomplete measurements. To handle this, we applied a combination of mean imputation and K-nearest neighbor (KNN) imputation, choosing the method based on the characteristics of the missing data. KNN is particularly effective when the missing value is assumed to be similar to neighboring instances in the feature space [27].

Following imputation, feature engineering is applied to enhance the model's ability to detect patterns in the data. Features related to the process, such as material properties and machine settings, are aggregated through sliding windows, calculating moving averages and standard deviations, to capture trends and temporal dependencies in the production process. Such transformations are critical because semiconductor manufacturing involves dynamic processes, where conditions evolve over time and are influenced by a multitude of interacting factors.[28]

Normalization is performed on the features to standardize the data before feeding it into machine learning algorithms. Z-score normalization is applied, as this approach is well-suited for algorithms like Support Vector Machines (SVM) and K-Nearest Neighbors, which are sensitive to differences in the scale of the input features.[29]

3.2 xAutoML Framework for Defect Prediction

The central component of the methodology is the xAutoML framework, which automates key steps in the machine learning process and integrates explainability techniques to ensure the model's predictions are interpretable. The goal of the framework is to enable high-quality defect prediction in semiconductor manufacturing while offering transparency into the decision-making process. The steps involved in the xAutoML framework are detailed below, which include feature engineering, model selection, hyperparameter tuning, and evaluation, each of which plays a crucial role in achieving the study's objectives.

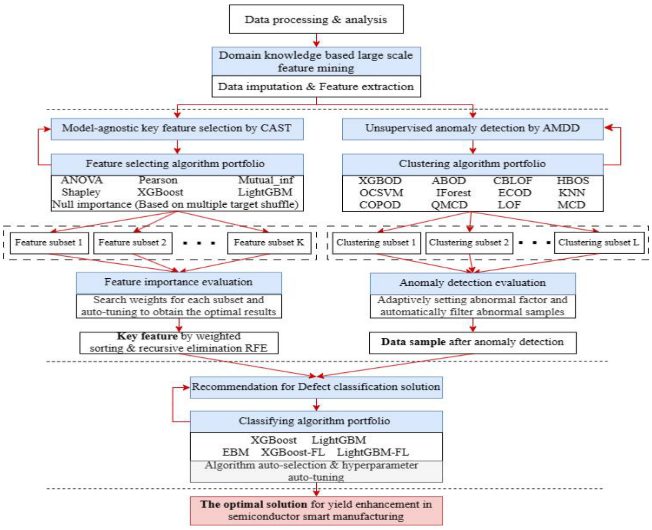

Figure 1: xAutoML Framework Diagram

3.2.1 Feature Engineering and Selection

Feature engineering is the first step in the xAutoML pipeline. Given the high-dimensional nature of semiconductor data, domain knowledge is leveraged to identify critical process parameters that are most likely to influence defect occurrence. These include parameters such as temperature, pressure, and material quality, which are derived from the production process and known to affect wafer quality. After extracting these raw features, additional derived features are created, such as moving averages and sliding windows, to capture temporal dependencies and variability over time.

Following feature engineering, feature selection is performed to reduce the dimensionality of the dataset and improve the efficiency of the machine learning models. In this study, a model-agnostic feature selection technique specifically, Recursive Feature Elimination (RFE) is employed. RFE systematically eliminates less important features by recursively fitting models and selecting the most relevant features that improve the performance of the machine learning model. This is particularly important in semiconductor defect prediction, where irrelevant or redundant features may not contribute to model accuracy but

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can increase computational complexity.

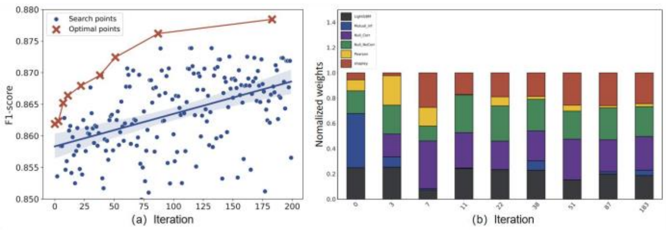

FIGURE 2: CAST FEATURE SELECTION PERFORMANCE

3.2.2 Model Selection and Hyperparameter Optimization

Once the relevant features are selected, the next step in the xAutoML framework is to automatically select the best-performing model and optimize its hyperparameters. This process involves iterating over a variety of machine learning algorithms, including Random Forests (RF), Support Vector Machines, XGBoost, and Gradient Boosting Machines (GBM). Each of these models has strengths in different aspects of defect prediction. For example, RF is a versatile ensemble method that works well with high-dimensional data and non-linear relationships, while XGBoost and GBM are more effective at handling structured data with complex interactions between features.

To automate the selection and tuning of hyperparameters, Bayesian Optimization (Snoek et al., 2012) is employed. This technique models the performance of hyperparameter configurations as a probabilistic function and uses previous iterations to guide the search for optimal hyperparameters. The goal is to minimize the cross-validation error and find the hyperparameter settings that yield the best performance, with fewer evaluations compared to traditional grid or random search approaches.

The Bayesian optimization process can be expressed as:

$$\theta^* = \arg\min_{\theta}[\mathbb{E}[\mathcal{L}(f(\theta))]]$$

where θ^* is the optimal hyperparameter set, $\mathcal{L}$ is the loss function, and $f(\theta)$ represents the model's performance given the hyperparameter configuration θ.

3.2.3 Model Evaluation

Model evaluation is crucial to ensuring that the final model performs well in real-world scenarios. Since the semiconductor defect prediction problem involves imbalanced data, where defective samples are rare, standard evaluation metrics like accuracy may not provide a true reflection of the model’s performance. For this reason, precision, recall, and F1-score are prioritized, as they better capture the trade-off between detecting defects and minimizing false positives.

Accuracy: The proportion of correctly predicted instances.

$$\text{Accuracy} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{TN} + \text{FP} + \text{FN}}$$

Precision is calculated as:

$$\text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}}$$

where TP = True Positives and FP = False Positives.

Recall, which is also known as sensitivity or the true positive rate, is given by:

$$\text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

where FN = False Negatives.

F1-score is the harmonic mean of precision and recall, providing a balanced metric for imbalanced classification problems:

$$\text{F1} - \text{Score} = 2 \times \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$$

To evaluate the model’s performance, stratified k-fold cross-validation is used, ensuring that each fold maintains a similar distribution of defective and non-defective samples. This method helps address the bias introduced by data imbalance and provides a more accurate estimate of the model’s generalization capability.

$$\text{Focal Loss} = -\alpha_t(1 - p_t)^{\gamma}\log(p_t)$$

SMOTE: A technique for generating synthetic examples of the minority class by interpolating between existing defective samples. This helps balance the dataset and provides the model with more information about the characteristics of defective units.

3.3 CHALLENGES AND ADJUSTMENTS

During the implementation of the xAutoML framework, several challenges arose. One notable challenge was the limited availability of labeled defect data, which prompted the use of simulated defect data to augment the dataset. While this allowed for a more comprehensive analysis, it also introduced potential biases, as synthetic data may not perfectly reflect real-world conditions.

Another challenge was the computational complexity of integrating explainability techniques such as SHAP and LIME. Although these tools provide valuable insights, they require significant computational resources, particularly when applied to large datasets. Future research may explore ways to optimize these techniques to improve real-time model performance.

4 EXPERIMENTS

This section presents the experimental setup used to evaluate the performance of the xAutoML framework for defect prediction in semiconductor manufacturing. The experiments were designed to assess the framework's ability to handle key challenges such as model selection, hyperparameter optimization, data imbalance, and the need for interpretability. By automating the process of model selection and integrating advanced techniques for explainability, the xAutoML framework aims to provide a

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robust solution to semiconductor defect prediction while ensuring that the resulting predictions can be trusted and understood by domain experts. The section includes details on the experimental design, model evaluation metrics, and the results obtained from applying the framework.

4.1 Experimental Design

The primary goal of the experimental setup was to evaluate the xAutoML framework's ability to predict semiconductor defects with high accuracy and interpretability. This required overcoming challenges such as small and imbalanced datasets, where defective wafers are rare, and ensuring the model's decisions could be explained to manufacturing engineers.

4.1.1 Data Splitting and Cross-Validation

Given the limited size of the available defect data, the dataset was split into 80% training, 10% validation, and 10% testing subsets. To ensure robust model performance and reduce overfitting, stratified k-fold cross-validation was employed. Stratified cross-validation helps to maintain the same proportion of defective and non-defective samples in each fold, which is critical given the severe class imbalance in defect prediction tasks. This method provided a more reliable estimate of model performance and helped mitigate the risk of bias towards the majority class.

4.1.2 Model Selection and Hyperparameter Tuning

In line with the xAutoML framework, multiple machine learning models were considered for defect prediction. These included Random Forests, Support Vector Machines, XGBoost, and Gradient Boosting Machines, each known for its ability to handle complex, non-linear relationships within data. A key feature of the framework is the automation of model selection and hyperparameter optimization, which was achieved using Bayesian optimization. This approach iteratively searched for the optimal combination of hyperparameters, minimizing cross-validation error and reducing computational cost.

4.1.3 Handling Data Imbalance

Since semiconductor defect data is typically imbalanced, with defective samples being much less frequent than non-defective ones, addressing this imbalance was crucial to ensure that the model could accurately predict defects. The xAutoML framework incorporated two key techniques to handle data imbalance:

Focal Loss, which modifies the standard cross-entropy loss function by focusing more on hard-to-classify instances, helping the model to pay more attention to the minority class.

SMOTE, which generates synthetic samples for the minority class by interpolating between existing defective instances. This increased the number of defective samples available for training and helped balance the dataset.

These techniques were integrated into the training process to improve the model's ability to detect defects, despite the imbalanced nature of the data.

4.1.4 4.1.4 Evaluation Metrics

The performance of the model was evaluated using several key metrics, given the imbalanced nature of the defect prediction task:

Accuracy: The proportion of correctly predicted instances namely, the true positives and true negatives.

Precision: The proportion of true positive predictions out of all predicted positives.

Recall: The proportion of true positive predictions out of all actual positives, emphasizing the need to identify defects correctly.

F1-Score: The harmonic mean of precision and recall, providing a balance between detecting defects and minimizing false positives.

Confusion Matrix: A detailed matrix showing the counts of true positives, false positives, true negatives, and false negatives, offering a comprehensive view of model performance.

Recall was given particular importance due to the nature of semiconductor manufacturing, where missing a defect could lead to significant quality issues. Stratified k-fold cross-validation was used to ensure that the evaluation was conducted on balanced subsets of data, helping to avoid bias towards the majority class.

4.2 Experimental Results

The results presented below provide an overview of the performance of the xAutoML framework in predicting defects in semiconductor manufacturing. These results are analyzed from multiple perspectives, including the impact of different machine learning models, the effectiveness of the imbalance handling techniques, and the interpretability of the model's predictions.

4.2.1 Model Performance

The xAutoML framework automatically selected the best-performing models and optimized their hyperparameters using Bayesian optimization. The performance of each model was evaluated based on the metrics outlined above. The results, as shown in Table 1, illustrate the effectiveness of the models in terms of accuracy, precision, recall, and F1-score:

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TABLE 1: PERFORMANCE COMPARISON OF MACHINE LEARNING MODELS FOR SEMICONDUCTOR DEFECT PREDICTION

Model	Accuracy (%)	Precision (%)	Recall (%)	F1-Score (%)
Random Forest	92.5	90.2	88.7	89.4
Support Vector Machine	91.8	89.5	85.9	87.7
XGBoost	93.2	91.0	90.1	90.5
Gradient Boosting	92.0	90.8	87.4	89.0

As seen in the table, XGBoost emerged as the best-performing model in terms of both F1-score and recall, demonstrating its ability to handle the imbalanced defect data effectively. While Random Forest and SVM also performed well, XGBoost exhibited the best balance between precision and recall, making it the most effective model for this task.

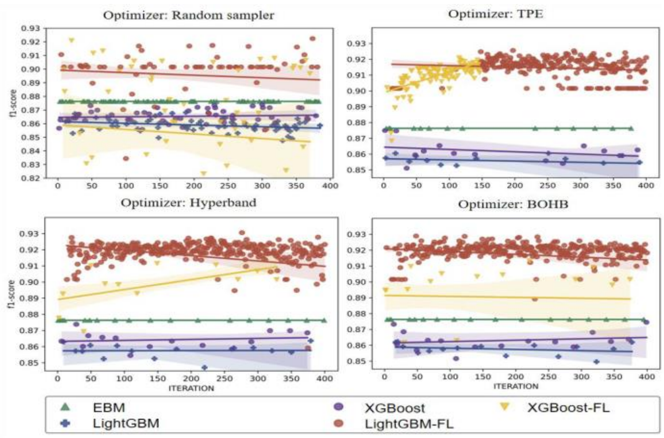

FIGURE 3: CLASSIFIER PERFORMANCE WITH OPTIMIZERS

4.2.2 Effectiveness of Data Imbalance Solutions

The impact of addressing data imbalance was significant in improving model performance. When no imbalance handling techniques were applied, the models struggled to detect defects, as the majority class dominated the learning process. Table 2 shows the performance of models without the use of focal loss and SMOTE, illustrating the improvement in recall and F1-score when these techniques were applied:

TABLE 2: RECALL IMPROVEMENT WITH IMBALANCE HANDLING TECHNIQUES

Model	Recall without Imbalance Handling (%)	Recall with Imbalance Handling (%)	Improvement (Percentage Points)
Random Forest	75.2	88.7	+13.5
Support Vector Machine	72.1	85.9	+13.8
XGBoost	78.4	90.1	+11.7
Gradient Boosting	74.5	87.4	+12.9

As indicated by Table 2, both focal loss and SMOTE contributed significantly to improving recall across all models, confirming that these techniques were effective in handling the class imbalance. By generating synthetic defective samples and adjusting the loss function, the models became better at identifying rare defects.

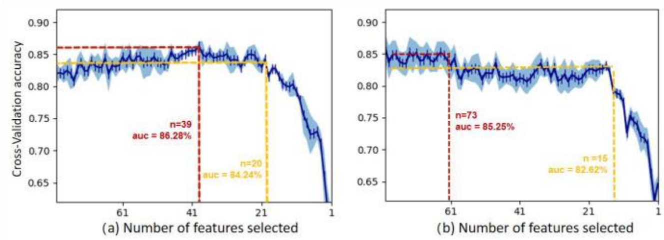

FIGURE 4: RFE PROCESS COMPARISON

4.2.3 4.2.3 Explainability and Interpretability

An essential component of the xAutoML framework is its ability to provide explainable predictions, which is crucial for decision-making in semiconductor manufacturing. Through the integration of SHAP and LIME, the framework provides insights into the factors influencing defect predictions, enhancing the model's transparency and trustworthiness.

SHAP values revealed that key process parameters, such as temperature and pressure, were consistently identified as the most influential features in predicting defects. For example, higher temperature levels were strongly associated with defects in wafer surface quality, suggesting that maintaining optimal temperature control could help reduce defect rates.

LIME was also used to provide local explanations for individual predictions, particularly for edge cases or anomalies in the data. This allowed engineers to understand why a particular wafer was predicted to be defective, offering

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actionable insights for process adjustments.

4.3 Discussion

The experimental results indicate that the xAutoML framework is a promising solution for semiconductor defect prediction. The integration of automated model selection, hyperparameter tuning, and data imbalance handling techniques provided a robust and effective model for predicting defects, with XGBoost emerging as the top-performing model. The recall improvements seen with the application of focal loss and SMOTE further highlight the importance of addressing data imbalance in defect prediction tasks.

The incorporation of explainability through SHAP and LIME enhances the practical value of the framework by providing domain experts with insights into the key factors driving defect predictions. This transparency is crucial for decision-making in industrial settings, where the ability to act on predictions is as important as the accuracy of the predictions themselves.

However, it is important to note that the results are based on publicly available and simulated data, which may not fully capture the complexities of real-world semiconductor production. Future work is needed to integrate real-time sensor data and extend the feature set to include more detailed process parameters. Additionally, the computational overhead of explainability techniques like SHAP and LIME may limit their scalability in real-time industrial applications. Further optimization of these techniques will be necessary to enhance their efficiency.

4.4 Conclusion of Experimental Results

In conclusion, the xAutoML framework offers a powerful solution for predicting semiconductor defects, addressing the challenges of model selection, data imbalance, and interpretability. The promising results demonstrated by the XGBoost model, alongside the improvements in recall and F1-score through the integration of focal loss and SMOTE, highlight the effectiveness of the framework. The incorporation of SHAP and LIME further underscores the framework's practical applicability by providing transparency and enabling actionable decision-making. While the current experiments provide a solid foundation, further research is needed to incorporate real-time data and optimize explainability techniques for large-scale industrial applications.

5 CONCLUSIONS

This study presents a novel xAutoML framework for semiconductor defect prediction, designed to automate key stages of the machine learning pipeline while addressing challenges such as data imbalance and the need for model interpretability. The experimental results demonstrated that the framework, particularly through the use of XGBoost, achieved promising performance in terms of recall and F1-score, highlighting its ability to identify defects despite the imbalanced nature of the data. Furthermore, the integration of focal loss and SMOTE helped mitigate the impact of class imbalance, improving the model's sensitivity to the minority class. Importantly, the incorporation of explainability techniques such as SHAP and LIME added significant value, providing transparency in the model's decision-making process, which is critical in industrial applications where actionable insights are paramount.

However, the study also encountered several limitations. The reliance on simulated defect data and publicly available datasets may not fully capture the complexities of real-world semiconductor manufacturing environments. Moreover, while the xAutoML framework provides a robust solution, the computational cost associated with explainability methods such as SHAP and LIME could limit their scalability in real-time applications. Future work should focus on incorporating real-time data, improving the scalability of explainability techniques, and exploring additional feature engineering methods that might further enhance the model's performance in industrial contexts. Additionally, further research is needed to refine the framework's ability to adapt to the dynamic conditions of semiconductor production, including the integration of online learning techniques for continuous improvement as new data becomes available.

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The original contributions presented in the study are included in the article/supplementary material, further inquiries can be directed to the corresponding author.

CONFLICT OF INTEREST

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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AUTHOR CONTRIBUTIONS

Not applicable.

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