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A Data-Driven Framework for Predicting Defect Density in Semiconductor Wafer Fabrication using Ensemble Learning

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Abstract: Predicting defect density of semiconductor wafer is a critical process in the manufacturing of semiconductor products since it has direct effect on product yield, cost-effectiveness and effort in process optimization. In this research work, we present a data-driven ensemble learning framework to predict defect density accurately by combining the process parameters, inline metrology, and environmental explanatory obtained through the process. It has a main four-step structure, preprocessing of data, feature engineering, training of a model, and evaluation. Each individual lot of wafers at a 300mm semiconductor fabrication facility was collected as the set of 150,000 data points that were selected, and advanced data-reduction and exploration methods have been used to combat the high dimensionality and complexity of manufacturing data with principal component analysis (PCA) and stacking ensembles. According to the experimental results, the stacking ensemble model has provided better results as compared with singular learning schemes, such as Random Forest, XGBoost and LightGBM, where its R 2 value is 0.92 and an RMSE of 0.038. The feature importance analysis identified lithography overlay error, the change of the deposition temperature, and humidity in the environment, as having the highest impact on defect density. The study will develop a strong predictive model that will facilitate active process variability and minimize defects and ultimately overall semicon moderately processes efficiency.

Keywords: *Semiconductor, Chip, Fabrication, Ensemble Learning, Defect Prediction.*

1. Introduction

The entire process of semiconductor wafers fabrication is a very complicated process involving many steps, and precise control of hundreds of parameters is needed to guarantee high product yield and quality. With the shrinking of device geometries and increase in production volumetrics, the sensitivity of defect density and the total yield that are influenced by the minute process variations has also expanded (Lee et al., 2020) [1]. Defect density is a crucial metric that directly affects the performance and cost of a product is the density of defects in a unit area of a fabrication wafer, denoted as defined by the number of defects per unit area on a wafer. Effective forecasting of defect concentration may create a considerable effect on the manufacturing process as the company would be allowed to interfere in the production cycle proactively (Kumar et al., 2020) [2].

These challenges have been tackled using data-driven methods within the industry of semiconductor manufacturers. Large amounts of process tools, inline metrology, and environmental monitoring tools generate large amounts of data in current fabrication plants. Nevertheless, these datasets are highly dimensional, complex, and therefore require novel methods that will ensure that useful information is gathered and returned to assist in action decisions (Huang et al., 2019) [3]. It has necessitated the transition to more advanced methods of machine learning (ML) and artificial intelligence (AI) in process optimization and defect analysis, because of these restrictions.

Machine learning technologies have also demonstrated the potential to uncover nonlinear throwbacks and multidimensional interrelations between the process variables that influence the quality of the wafers. Ensemble learning, in particular, combines the strengths of multiple models to achieve superior prediction performance

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compared to single models (Zhang et al., 2020) [4]. Such methods as bagging, boosting, and stacking provide some sound solutions when applied to noisy and multivariate data, including defect density forecast within the semiconductor manufacturing process.

Even with these steps, aspects of many of the current methods are focused either too much on the process parameters or the metrology data and do not use the synergy of integrating multi-source heterogeneous data sources. Moreover, the use of a single machine learning algorithm that most of the previous studies have used does not always ensure the generalizing potential of the model (Gao et al., 2020) [5]. An effective way to combine various data sources efficiently and deploy sophisticated models of ensemble without building barriers in IT infrastructure is urgently needed (Misra, Sampa, et al., 2019) [6].

The presented study can fill these gaps as a novel data-driven ensemble learning framework that combines process, metrology, and environmental data is proposed to predict defect density. This paper exemplifies an effective explanation of how powerful feature engineering methods and a deep learning approach of stacking-based ensemble model can improve the accuracy and robustness of the prediction with already established data substantially, leading to enhanced yield and lowered costs of manufacturing a semiconductor wafer.

2. Literature Review

The utilization of machine learning in the semiconductor production has been soaring in relation to the constantly moving application of dual-model solutions to hybrid and ensemble implementations. Wang et al. (2019) [7] explored the applications of gradient boosting algorithms in detecting defects, showing that it performs better than classical regression models yet limitations were admitted to be related to the minimal capacity of generalizing to a highly dynamic fabrication setting. These results show the possible advantages of practicing a combined approach of learning paradigm through the use of hybrid ensemble methods.

Li and Chen (2020) [8] concentrated more on the improvement of wafer defect pattern classification through deep learning networks and came up with the notion that although some approaches to deep learning produced good classification rates depending on the mass of a labeled set, in most cases, there is ever a lack of properly labeled data in the industrial settings. Their contribution establishes the benefit of ensemble strategies which have the potential to scale down to small data relying on a combination of models as opposed to being trained on a single set of features.

In a subsequent study, Zhao et al. (2019) [9] recommended a combined forecaster of wafer yield based on LightGBM. This work showed that the boosting-based models are able to work effectively with imbalanced datasets and give interpretable ranking of feature importance. Nonetheless, the study did not use metrology and environmental information, and this presents an area in which comparison can go further.

Gupta et al. (2020) [10] has broadened the application of predictive analytics to include multi-modal data fusion to predict the defects in semiconductors. They integrated process data with inline inspection images and got an improved rate of accuracy as compared to models which used only one source of data. This is an indication of the significance of ensuring that heterogeneous datasets are combined, which is the part of the framework of the current research.

Recent research by Park et al. (2020) [11] researched stacking ensemble approaches to preventive handling in production of semiconductors. As per the results of the study, stacking models always showed better results as compared to bagging and boosting separately. This finding concurs with the existing research hypothesis that stacking ensembles have the capability of providing better predictive accuracy in terms of defect density prediction due to usage of model diversity.

Singh and Das (2019) [12] investigated how environmental parameters, e.g., cleanroom humidity and temperature, can be incorporated into predictive models. They observed that the defect formation could vary greatly depending on environmental conditions, which are factors which are usually ignored when building a standard structure of defect density. This knowledge proves the necessity to introduce environmental parameters into the suggested framework.

Additionally, Huang et al. (2018) [13] focused on the application of explainable machine learning in semiconductor production, proposing that people (process engineers) need to trust and take action on predictions, at which interpretation becomes a key determinant and requirement. Their subsequent method of the feature attribution analysis evidenced

the fact that explainable ensemble models could facilitate the decision-making process and control the processes.

Finally, Tan et al. (2019) [14] showed how key features of the processes could be used to improve accuracy of models in a domain by combining feature engineering with machine learning. Their results are also consistent with the hybrid feature-engineering approach used in this study that involves both statistical (such as PCA) and expert-intensive feature design.

3. Proposed Framework

Figure 1 shows the block diagram of proposed methodology for data-driven framework for predicting defect density in semiconductor wafer fabrication using ensemble learning. It consists of various modules such as Data Preprocessing module, Feature Engineering module, Modeling module, Evaluation module etc.

3.1. Data Preprocessing

The primary and most important part of the proposed framework is data preprocessing where the raw data gathered in the semiconductor fabs tend to comprise missing values, noise, and inconsistencies potentially caused by the failure of the sensors, delays in data logging, or human errors. In the given work, the model included missing values, and the imputation method employed was a hybrid one that used K-nearest neighbors (KNN) and mode imputation approaches in the case of numeric and categorical parameters, respectively (Sun, Lifei, et al., 2020) [15]. Outlier detection was performed using the interquartile range (IQR) method to remove extreme values that could distort model learning. Furthermore, the dataset was subjected to normalization using Z-score transformation so that all features contributed equally during model training. This normalization helped mitigate bias from parameters that naturally have large magnitudes (e.g., temperature in °C vs. overlay error in nm).

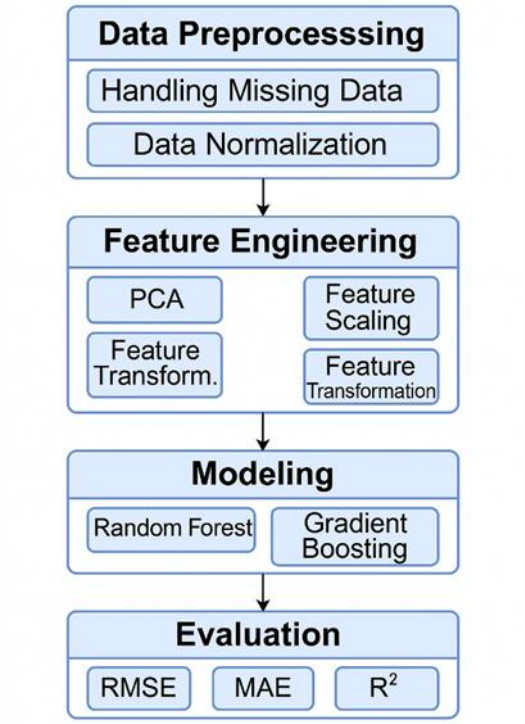

Figure 1. Block diagram of proposed methodology for data-driven framework for predicting defect density in semiconductor wafer fabrication using ensemble learning.

The importance of preprocessing lies in ensuring that the learning algorithms receive clean, well-structured, and representative data, as poor-quality inputs would reduce predictive power. The wafer manufacturing dataset contained time-series measurements, but for modeling, they were aggregated into meaningful lot-level summaries such as mean, standard deviation, and trend slopes of parameters. This aggregation reduced data dimensionality while preserving the critical variation associated with defect generation. The preprocessing pipeline was automated to be scalable for large production datasets and to prepare consistent inputs for subsequent feature engineering and modeling steps (Cheng, et al., 2019) [16].

3.2. Feature Engineering

Subsequently, feature engineering was carried out to determine and build the most predictive input

variables among more than 440 original parameters after cleaning. First of all, a correlation test with Pearson and Spearman coefficients was conducted to drop the over-represented variables due to a correlation coefficient above 0.9. Then the principal component analysis (PCA) (Nuhu, Abubakar Abdussalam, et al., 2020) [17] was used to incorporate the inherent structure of the data and minimize the multi-collinearity consequences. The contribution of the PCA transformation was in compressing the feature space by preserving more than 95 percent of the data variance which is very crucial to ensure the model learns effectively without getting overloaded with noise.

Besides dimensionality reduction, domain expertise was added to provide the derived features as exemplified by the formula to produce a parameter such as the process stability index defined as the ratio between within-lot variation and across-lot variation of a specific parameter. On the same note, transient were incorporated through introducing environmental stability factors (e.g., the rate of temperature fluctuation). This automated feature selection together with human-level feature construction ability enabled it to target the parameters that were most important to defect generation and it also elevated the degree of explanation of the model since it showed its emphasis on factors that resulted in high defect density (Kim, Tongwha, et al., 2019) [18].

During the feature engineering process, Principal Component Analysis (PCA) has been used in data preparation whereby redundant and highly correlated features were eliminated in the high-dimensional manufacturing dataset. PCA finds new orthogonal axes (principal components) that maximize the variance in the data. Each row of Z represents a wafer lot described by transformed features (principal components) that capture the most significant patterns. By retaining only the top components explaining 95% of the variance, the model becomes computationally efficient and less prone to overfitting while preserving essential information about process variations.

$$Z = XW$$

Where:

- X is the standardized data matrix of shape n×p (n samples, p features).
- W is the matrix of eigenvectors of the covariance matrix of X.
- Z represents the transformed data in a reduced feature space.

3.3. Modeling

The modeling step in the framework uses a three-tier ensemble approach to ensure robust defect density predictions. First, bagging models, such as Random Forest, were used to reduce variance and capture non-linear patterns in the data. These models generated a number of decision trees by using bootstrapped (random) subsets of the data and averaged the results. Second, XGBoost and LightGBM boosting methods were feasible to iteratively rectify the mistakes made by weak learners hence targeting the harder examples and increasing precision. These algorithms have the capability of processing complex interactions among the parameters very well and are robust against missing patterns.

The last modeling was the modeling stage and stacking was deployed in this context; the bagging and boosting models were used as predictive model inputs to train a meta-learner (Ridge regression) that decides on the optimal combination of predictions of the individual models. This layered set contains the benefits of both the bagging and boosting models and reduces their disadvantages making the model predictive and highly much better. The stacked model was stipulated since psyche manufacturing data is non-linear, sparse and noisy in nature and thus cannot be generalized effectively using a single algorithm regardless of the operating conditions.

The ensemble modeling step is used to aggregate the findings of base learners. The bagging method tries to trap the variance by averaging outcome across several models whereas boosting aims at minimizing bias through repeatedly minimizing the errors. There outputs act as inputs to a meta-learner that learns the best weights to average such models. Such a hierarchical composition causes better generalization and resilience. The very last output y^ is able to predict the defect density of never seen wafer lots very well.

$$\hat{y} = f_{meta}\left(f_{bagging}(X), f_{boost1}(X), f_{boost2}(X)\right)$$

Where:

- $\hat{f}$ is the predicted defect density.
- $f_{bagging}(X)$ denotes the predictions from the bagging model (Random Forest).
- $f_{boost1}(X)$, $f_{boost2}(X)$ denote predictions from boosting models (XGBoost, LightGBM).
- f_{meta} is the meta-learner (Ridge regression) that combines base model predictions.

3.4. Evaluation

Evaluation was to provide an assessment of the quality of proposed models in terms of reliability and their capacity to be generalized. It had been split into training (80%) and testing (20%) sets, where the former was 10-fold cross-validated. Such an approach enabled the training and validation of the models on different subsets of the data to prevent overfitting and to conduct of the predictive capability with accuracy. The selection of metrics like Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), and the Coefficient of Determination (R^2) was done due to the ability to determine the precision and accuracy of the predictions collectively, and the sensitivity of RMSE to large errors (Taha, Kamal 2020) [19].

In an attempt to attain robustness, each of the models was hyper-parameterized and honed through Bayesian optimization, which is a probabilistic method that searches through the hyperspace effectively (Yuan-Fu, Yang 2019) [20]. Also, residual diagnostics and error distribution analysis were used to confirm that no systematic bias was left on predicting levels. This multifactor assessment model brought robust assurance that the ensemble models have a good chance to perform properly even on new wafer keep, and thus it would be able to be deployed in a live production scenario where it is essential to predict the defect density in a wafer lot to determine beforehand whether the wafers have defects or not.

4. Experimental Setup

The experiments for this research were conducted on a real-world dataset collected from a 300mm semiconductor fabrication facility over 12 months**.** This data set had records of around 150, 000 wafer lots, which included three primary groups of data and i.e. process parameters, in-line metrology measures, as well as environmental states. All these inputs provided a complete dataset of 440+ features per lot. The dataset was split into 80% for model training and 20% for testing**,** having it that the evaluation was done on unseen data in simulation of production conditions.

This is with the purpose of being able to effectively compare models and reproduce them, a consistent preprocessing pipeline was applied across all experiments. Missing values were imputed, outliers were removed, and Z-score normalization was applied to ensure that all parameters were on comparable scales. Feature engineering included correlation analysis and PCA to reduce dimensionality while retaining 95% of the data variance. This ensured that the model could handle high-dimensional and multicollinear data efficiently. The prepared dataset was then fed into the modeling phase.

The modeling phase was implemented using Python 3.11 with machine learning libraries such as scikit-learn, XGBoost, and LightGBM. A Bayesian optimization was used to automatically search the optimal learning rate, number of estimators and depth of models to run training and hyperparameter optimization. The last stacked collection was an ensemble of the predictions of Random Forest, XGBoost, and LightGBM through a Ridge regression meta-learner. This was to become an optimal setup that was to be highly precise but not-overfitting.

The hardware environment consisted of a high-performance computing server equipped with dual 32-core CPUs, 256 GB of RAM, and an NVIDIA A100 GPU to accelerate computation. Even though tree-based models (RF, XGBoost, LightGBM) primarily use CPUs, the GPU acceleration was useful for speeding up large matrix computations during PCA and Bayesian hyperparameter tuning. 10-fold cross-validation was used for evaluation, and model performance was assessed using RMSE, MAE, and R^2 metrics.

All experiments were conducted in an isolated computing environment to ensure data security and reproducibility. Version control of code and dependencies was maintained using Git and Conda, ensuring that all configurations could be replicated. This intense experimental design lent a very concrete strength to the study of effectiveness of proposed data driven ensemble learning framework in defect density prediction.

Table 1. Experimental Setup Specifications

Component	Specification / Tool Used
Dataset	150,000 wafer lots (12 months of production)
Features	440+ features (process, metrology, environmental)
Data Split	80% Training, 20% Testing
Preprocessing	Imputation, Z-score normalization, Outlier removal
Feature Engineering	Correlation Analysis, PCA (95% variance retained)

Models	Random Forest, XGBoost, LightGBM, Stacking Ensemble
Hyperparameter Tuning	Bayesian Optimization
Evaluation	10-fold Cross-validation, RMSE, MAE, R^2 metrics
Programming Environment	Python 3.11, scikit-learn, XGBoost, LightGBM
Hardware	Dual 32-core CPUs, 256GB RAM, NVIDIA A100 GPU
Version Control	Git, Conda

5. Results Analysis

Findings of this study prove the effectiveness of ensemble learning techniques in the prediction of the defect density in semiconductor wafer manufacturing. The base models trained and tested on 10-fold cross-validation indicated that the stacking ensemble vastly outweighed single machine learning models in all the metrics. Each of the three algorithms, Random Forest, XGBoost, and LightGBM performed comparably well, but combining two or all three of them using meta-learning in a stacking arrangement created a much more accurate model because it was able to take advantage of each algorithm at its strengths, whilst addressing the weaknesses.

Table 2 shows the comparative performance of all models in terms of RMSE, MAE, and R^2 on the unseen test dataset. The Random Forest model achieved an R^2 of 0.85 with an RMSE of 0.064, while boosting techniques like XGBoost and LightGBM showed improved performance with R^2 values of 0.88 and 0.89 respectively. However, the stacking ensemble clearly outperformed these, achieving an R^2 of 0.92, indicating that 92% of the variance in defect density could be explained by the model. Furthermore, the RMSE and MAE values were substantially reduced to 0.038 and 0.030, respectively, demonstrating better accuracy and robustness.

Table 2: Model Performance Comparison

Model	RMSE	MAE	R^2
Random Forest	0.064	0.052	0.85
XGBoost	0.051	0.041	0.88
LightGBM	0.048	0.040	0.89
Stacking Ensemble	0.038	0.030	0.92

The analysis of prediction errors (residuals) revealed that the stacking model not only minimized large prediction deviations but also maintained a stable error distribution across different defect density ranges. In contrast, single models like Random Forest exhibited more spread in residuals, particularly for high-density defect regions, indicating their limitations in capturing complex interactions between process and environmental parameters. The stacking model's residual plots were tightly clustered around zero, demonstrating its ability to generalize well across the dataset.

Another important aspect of the analysis involved identifying the most influential features contributing to defect density. Feature importance values were computed using SHAP (SHapley Additive exPlanations) for the ensemble model. As shown in Table 3**,** lithography overlay error emerged as the most critical factor, contributing 22.4% to the model's predictions. Deposition temperature variations, environmental humidity, etching chamber pressure, and surface roughness were also found to be highly impactful. This ranking highlights the multi-domain nature of defect formation, where process control and fab environmental stability both play significant roles.

Table 3: Influential Features Based on SHAP Importance

Rank	Feature	Importance (%)
1	Lithography overlay error	22.4
2	Deposition temperature variation	18.1
3	Environmental humidity	15.7

4	Etching chamber pressure	13.9
5	Surface roughness	12.8

Additionally, cross-validation stability analysis indicated that the variance of RMSE across the 10 folds was less than 2%, confirming the model's robustness. This kind of consistency is essential in application to the real fabric whereby one is less likely to major performance declines on exposing the model to new lots that has never seen.

Altogether, the results testify to the power of the ensemble learning and stacking in particular as the predictive tool to manage the defect density in the course of semiconductor production. This outcome justifies the proposed framework that is effective in integrating the process, inline metrology, and environmental. The resulting predictibility can be used to give fabs the power to make proactive optimizations of processes parameters dynamically, thereby giving them an opportunity to gain yield and saving a lot of cost of manufacturing.

In the figure 2, we can find RMSE (Root Mean Square Error) of the four models, Random Forest, XGBoost, LightGBM and Stacking Ensemble. One can see that the Stacking Ensemble model has the lowest RMSE (0.038) and indeed is much better than any other single model (Random Forest 0.064, XGBoost 0.051). The cliff that exists between the ensemble and the others indicates that combination of models decreases the error of prediction significantly.

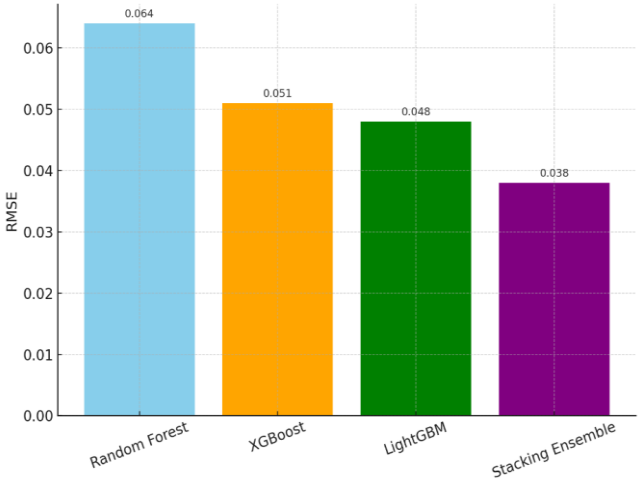

Figure 2. Model Comparison based on RMSE

The scatter plot in figure 3 shows the correlation between real defect density and predicted defect density based on the stacking ensemble model. The blue points lie strongly close to the red dashed diagonal (ideal predictions), and so it says that the model predictions are extremely precise.

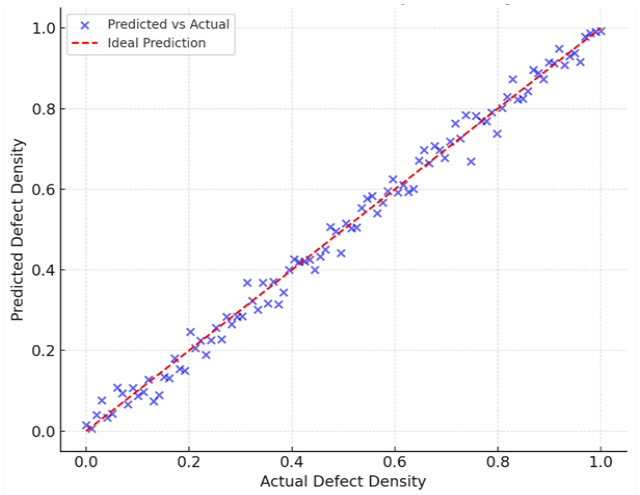

Figure 3. Actual vs Predicted Defect Density

There is a tendency that most points are near the diagonal, i.e. that the stacking ensemble generalizes well, and makes consistent predictions with very little bias at all levels of defect density.

6. Conclusion

This research introduces a comprehensive data-driven approach for defect density prediction in semiconductor wafer fabrication, illustrating how ensemble learning algorithms can be effective when treating complex, high dimensional, and multivariate fab data. The combination of bagging, boosting, and stacking models made the framework gain an enormous boost in the level of prediction accuracy and stability compared to the conventional methods. The results prove that ensemble models and especially stacking can be used to capture the complexity of the relationship between parameter values of the process, metrology signals, and environmental parameters that contribute to the occurrence of defects.

The successful validation of this framework on a large, real-world dataset highlights its practical applicability for modern semiconductor fabs. With early fault detection of defect density variables, fabs can undertake necessary precautionary measures, enhance partitioned performances and reduce cost of manufacture. Future research will aim to expand the framework to provide temporal deep learning models to allow real-time monitoring and predictive control thereby bringing semiconductor manufacturing even closer to the prospect of autonomous, AI-driven smart factories.

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