Human Interpretable Virtual Metrology in the Semiconductor Manufacturing

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Abstract

My PhD research focuses on developing a highly accurate and explainable multi-output virtual metrology system for semiconductor manufacturing. Using machine learning, we predict the physical properties of metal layers from process parameters captured by production equipment sensors. Key contributions include a model-agnostic explanatory method based on projective operators, providing insights into the most influential features for multi-output predictions and feature selection algorithms for these tasks.

Introduction

The rising demand for digitalization and decarbonization has led to the increasing production of chips (9.2 billion chips by Infineon Technologies AG in 2023 (Infineon Technologies AG 2023)), highlighting the need for faster, more reliable, and efficient semiconductor manufacturing with minimal waste. It is not always possible to fully inspect products during manufacturing due to the destructive nature of some testing techniques (Maitra, Su, and Shi 2024). The industry relies on random sampling and inspection, which does not ensure comprehensive quality control of products or optimal yields. With the growing use of artificial intelligence (AI), there is potential to predict product properties using data from existing monitoring systems. Key industry research questions include: *Which process control signals are necessary for accurate prediction of product properties? Which machine learning pipeline performs best and what metrics should be used to evaluate its performance?*

Virtual metrology (VM), introduced in 2005 in the semiconductor manufacturing industry (Chen et al. 2005), involves estimating a product's quality directly from production process data, using supervised or unsupervised machine learning (ML) algorithms (Yan et al. 2023), without physically measuring it (Maitra, Su, and Shi 2024), and in this way reducing production times and costs. The VM process is demonstrated in Fig. 1. Following the previous efforts in this direction (Maitra, Su, and Shi 2024), we focus on creating a VM system to predict the properties of a thin film produced in the physical vapor deposition (PVD) process. PVD is one of the main steps in the production process, and it is used to create thin metal layers by depositing metal vapor onto a substrate (Powell and Rossnagel 1999).

The important physical properties of the film, such as thickness and resistance, depend on process parameters like deposition time, power, voltage, electrical current, temperature, and pressure. After production, properties are measured at 17 points. We aim to predict both properties at all 17 points simultaneously, Fig. 1, which requires the use of methods suitable for predicting multiple variables.

Related Work

Multi-output learning is an ML paradigm that aims to predict multiple outputs simultaneously given an input (Xu et al. 2019). These methods improve prediction accuracy by capturing complex relationships between outputs, which is essential in scenarios with multiple interrelated factors. Multi-output approaches are overlooked in deep learning-based VM modeling, although the joint information among the process outputs can improve prediction performance. Only several scholars utilize these methods. Choi et al. (2024) proposed a CNN-based multivariate VM model us-

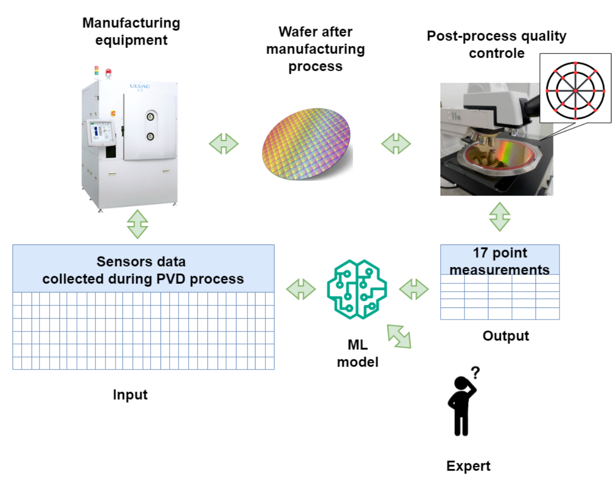

Figure 1: VM predicts wafer properties at 17 points using ML models and ensures informed decision-making regarding process adjustments and scheduling maintenance.

ing multi-sensor process sensor data and evaluated the proposed model for VM modeling at an etching process. Yamaguchi and Yamashita (2024) proposed a multi-target regression method that combines Random Linear Target Combinations and PCA. However, the inability to integrate such methods into production is due to a lack of transparency and explainability of the prediction process and its outcomes.

Production equipment sensors generate numerous signals, often aggregated into redundant variables. This requires feature selection and dimensionality reduction algorithms to be included as separate elements in VM systems. The process of feature selection is also a step toward explainability. Szedmak et al. (2023) proposed a novel approach for variable selection for vector-valued or two-view learning problems utilizing projection operators and their algebra - the Projective Selection (ProjSe) algorithm.

Although methods like SHAP (Kariyappa et al. 2024) and LIME (Ribeiro, Singh, and Guestrin 2016) address single-output interpretability, no approaches for multi-output explanations exist in the literature.

Objectives

My PhD aims to develop a predictive model, feature selection algorithm, and explanatory method for multi-output tasks. Its key contribution is a model-agnostic explanatory approach using projective operators, highlighting features critical for predicting multiple variables.

Results

During the first year, I focused on preprocessing data collected from semiconductor manufacturer and preparing the dataset for a multi-output prediction task. Additionally, I conducted a qualitative study with industry experts to understand processes, industry needs, and expectations from a predictive system. Existing single and multi-output prediction models were implemented and verified. ProjSe (Szedmak et al. 2023) algorithm was utilized to select and rank process parameters that are the most important for predicting product properties. Its stability was evaluated by comparing it with feature selection methods based on tree models. The results of feature selection aligned well with industry experts' experience and were consistent with the underlying physics of the process. These steps are building elements of the preliminary design of a VM system for predicting multiple physical properties of metal layers after the physical vapor deposition process.

In the second year, I developed the initial explanatory method grounded in the theory of the projective selection algorithm for vector-valued supervised learning problems (Szedmak et al. 2023). This approach is model-agnostic, ensuring wide applicability across various contexts. The effectiveness of the explanatory method has been successfully demonstrated on real-world datasets. Furthermore, I introduce a stability index to rigorously evaluate the reliability of the generated explanations. Our method outperforms SHAP and TreeInterpreter in computation time, while the introduced stability index and correlation are comparable.

Future Work

By the workshop date, I am planning to upgrade the explanatory method and, after the workshop, conduct qualitative and quantitative evaluations. This includes user studies with industry experts and testing the method on public datasets. Additionally, I aim to develop a feature selection method that is scalable and effective for various output dimensions since the ProjSe (Szedmak et al. 2023) performs well for around 20 outputs but struggles with fewer.

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