Predictive Modeling for Quantitative Compositional Engineering of InZnHfO Thin-Film Transistors

Jiho Lee[1] Serang Jung[1] Jungmin Gwon[2] Youn Sang Kim[1]

1Department of Chemical and Biological Engineering, College of Engineering, Seoul National University, Seoul, Republic of Korea

[2]Samsung Electronics, Pyeongtaek-si, Republic of Korea

Correspondence to: Youn Sang Kim younskim@snu.ac.kr

1. Introduction

Oxide semiconductors are essential for next-generation displays and flexible electronics due to their high mobility and excellent low-temperature processability. However, the vast and complex compositional space of quaternary systems like InGaZnO (IGZO) poses a significant challenge for fine-tuning electrical characteristics using traditional trial-and-error methods. To address this bottleneck, this study implements a machine learning (ML)-assisted approach to enable the quantitative optimization of oxide semiconductor. Specifically, the incorporation of Hafnium (Hf) into Indium-Zinc oxide (IZO) is adopted to control oxygen vacancies through Hf's strong oxygen bonding affinity. By combining the atomic-level precision of plasma-enhanced atomic layer deposition (PEALD) with the predictive power of ML algorithms, we aim to navigate the complete compositional range and identify optimal device performance with a minimal experimental dataset. This data-driven methodology builds upon our previous work demonstrating the effectiveness of Bayesian optimization and surrogate modelling in managing complex interdependencies within oxide thin-film transistors [1, 2].

2. Results and Discussion

The proposed framework follows a systematic ML workflow: (1) construction an initial experimental datasets of IZHO TFTs with varying In:Zn:Hf ratios using PEALD, (2) performing K-means clustering on transfer curves to categorize device behaviour, (3) building classification and regression models to map the relationship between chemical composition and electrical metrics, and (4) extracting optimal candidates through an acquisition function for experimental validation.

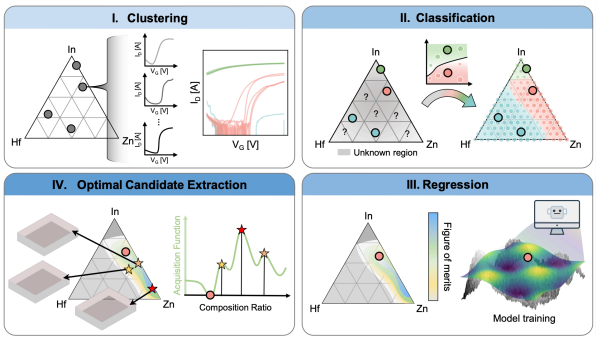

Fig. 1: Machine learning-assisted workflow for the quantitative optimization of InZnHfO TFTs.

In the modelling phase, we evaluated various algorithms, including Linear Regression (LR), Gaussian Process Regression (GPR), and eXtreme Gradient Boosting (XGBoost). The XGBoost and GPR models accurately predicted critical TFT metrics such as field-effect mobility, threshold voltage (V_{th}), subthreshold swing (S.S.), and on/off ratio. Regression analysis showed that GPR achieved the lowest root meand square error (RMSE) for most figures-of-merit. Furthermore, SHAP (Shapley Additive exPlanations) analysis was employed to interpret the contribution of each element (In, Zn, Hf) to the device performance, revealing the quantitative impact of Hf on electrical characteristics of TFTs.

By leveraging the predictive capabilities of the trained models, we identified an optimized IZHO systems that achieved outstanding performance, including a field-effect mobility exceeding 20 $cm^2/V{\cdot}s$ and a near-zero threshold voltage withing an ultra-thin channel thickness under 10 nm. These results represent a significant advancement in achieving simultaneous improvement of multiple electrical characteristics in ultrathin oxide TFTs, surpassing the performance limits often encountered in conventional optimized systems [3]. This work demonstrates that integrating PEALD with ML-enabled compositional engineering allow for efficient, scalable, and quantitative optimization of multi-component oxide semiconductors.

References

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