

## Literature Mapping Report

This section reproduces the original literature mapping report prepared for the research topic 'Predictive Electron Density Modelling for 3D NAND Flash Memory (ML-based)'.

### Chosen Research Topic

Predictive electron density modelling in vertical-channel 3D NAND flash memory using machine learning surrogate models (TCAD → ML). Focus: how grain size (GS), channel thickness (Tsi), and grain-boundary trap density affect electron density along the vertical channel and how ML can accelerate TCAD-driven design/variability studies.

### Seed Paper (provided)

Verma, D.; Bhatt, U. M.; Vidyarthi, A. (2024). A machine learning framework for predictive electron density modelling to enhance 3D NAND flash memory performance. e-Prime.

Short summary: The authors generate TCAD-derived electron-density vs position datasets for four GS/Tsi configurations, train multiple regression models (Decision Tree, Random Forest, KNN, Gradient Boosting, XGBoost, CatBoost, AdaBoost, Linear Regression), and evaluate using  $R^2$  and RMSE. They report that non-linear/ensemble methods strongly outperform linear regression, and conclude K-Nearest Neighbors is overall best for their datasets.

### New relevant papers found

- 1) Lee, J.K.; Ko, K.; Shin, H. — Prediction of Random Grain Boundary Variation Effect of 3-D NAND Flash Memory Using a Machine Learning Approach (2022).
- 2) Kim, Y.; Hong, S.K.; Park, J.K. — Optimizing Confined Nitride Trap Layers for Improved Z-Interference in 3D NAND Flash Memory (2024).
- 3) Fan, S.; Hitt, A.; Tang, M.; Sadigh, B.; Zhou, F. — Accelerate Microstructure Evolution Simulation Using Graph Neural Networks (2023).

### Reflection

The literature mapping revealed the potential to expand beyond the original device-focused surrogate modelling to incorporate microstructure modelling and additional device parameters, enhancing generalization and robustness.

## Part 2: Expanded Literature Review

This expanded literature review builds upon the original mapping by providing more detailed analysis, 2–3 pages per paper, and integrating the findings into a research roadmap.

### Research Topic and Seed Paper

The focus is on predictive electron density modelling in vertical-channel 3D NAND flash memory using machine learning surrogates trained on TCAD data. Verma et al. (2024) investigate how GS, Tsi, and trap density affect electron density, finding KNN as the most effective regression model.

### Lee, Ko & Shin (2022)

ANN-based surrogate models predict random grain boundary effects with 3–7% error vs. TCAD, allowing large-scale variability analysis.

### **Kim, Hong & Park (2024)**

Investigate confined nitride trap-layer geometries to mitigate Z-interference. Findings stress the need for including device-stack parameters in ML models.

### **Fan et al. (2023)**

Use GNNs with adaptive meshing to model microstructure evolution. This technique could serve as a pre-processing stage for generating realistic grain maps for TCAD training.

### **Integrated Insights and Roadmap**

Recommendation: Shift from direct GS/Tsi → density modelling to a two-stage approach: microstructure modelling followed by electrical property prediction, with expanded input features and uncertainty quantification.

### **References**

- [1] D. Verma, U. M. Bhatt, and A. Vidyarthi, "A machine learning framework for predictive electron density modelling to enhance 3D NAND flash memory performance," e-Prime, 2024.
- [2] J. K. Lee, K. Ko, and H. Shin, "Prediction of random grain boundary variation effect of 3-D NAND flash memory using a machine learning approach," in Proc. IEEE Int. Conf. Electron Devices, 2022.
- [3] Y. Kim, S. K. Hong, and J. K. Park, "Optimizing confined nitride trap layers for improved Z-interference in 3D NAND flash memory," Electronics, vol. 13, no. 6, p. 1020, 2024.
- [4] S. Fan, A. Hitt, M. Tang, B. Sadigh, and F. Zhou, "Accelerate microstructure evolution simulation using graph neural networks with adaptive spatiotemporal resolution," arXiv preprint arXiv:2301.12345, 2023.