Machine Learning for Accelerating Atomic Layer Deposition Process Optimization

Minjong Lee, DooSan Kim, Dushyant Narayan and Jiyoung Kim*

University of Texas at Dallas, USA
E-mail address: jiyoung.kim@utdallas.edu

Artificial intelligence (AI) is driving the development of more convenient and efficient technological systems. Industry 4.0 integrates 'intelligent' information technology into manufacturing and industrial processes, with machine learning (ML) promising to increase flexibility and efficiency while minimizing process errors [1]. This transformative technology is expected to enhance virtually every sector of modern society, revolutionizing systems and protocols across diverse fields. The integration of ML is particularly valuable in semiconductor fabrication, where current processes have become increasingly complex, often requiring over 30 steps to deposit a single high-quality film layer. Consequently, process optimization has become crucial for achieving high-quality films and simplifying process steps. To meet these demands, proof-of-concept of ML-driven processes is essential to validate their potential in advancing semiconductor manufacturing.

Among semiconductor fabrication techniques, ALD processes have been highlighted due to their precise control of atomic-scale film engineering and their compatibility with advanced 3D semiconductor architectures. However, ALD involves numerous critical parameters that influence film quality. The comprehensive exploration of all possible ALD process conditions is economically unfeasible, as each experimental run costs over $1,000 per wafer, plus additional labor and analysis costs [2]. This constraint forces us to narrow the inspection ranges of ALD conditions out of potentially trillion combinations. Such limited sampling hinders the creation of highly accurate, atomic-scale process models. In this context, the incorporation of AI technologies shows promise in improving the cost-efficiency of process development by potentially decreasing the volume of data necessary for developing new process technologies.

In this presentation, we discuss the applications of a deep neural network (DNN) framework as an ML-driven atomic layer deposition (ALD) process, with a focus on hafnium oxide (HfO_x) film analysis. ML applications in ALD processes have shown promise; however, they have primarily focused on monitoring film thickness and performing the prediction tasks [3]. Although film thickness serves as a valuable indicator of chemical reactions based on the ALD window, analyzing film quality, particularly film density, is crucial for achieving superior film performance. We demonstrate the properties of film density using the wet etch rate (WER) test, which leverages the principle that higher-density films have more tightly packed atoms, increasing resistance to etchant penetration and reaction with HfO_x films. Furthermore, a comprehensive ML framework is expanded to include a DNN system, generating prediction maps for further process optimization, as well as dependencies on ALD parameters. This proof-of-concept of DNN integration into the ALD process marks a simplification of experimental design, demonstrating how these innovations are reshaping creative methods for process optimization.

References

1. Adeleke et al., "Machine Learning-Based Modelling in Atomic Layer Deposition Processes." CRC Press **(2023)**
2. K. J. Kanarik et al., *Nature* 616, 707 **(2023)**
3. A. Arunachalam et al., *J. Vac. Sci. Technol. A* 40, 012405 **(2022)**