(Supplemental Document) Integrating Machine Learning into Atomic Layer Deposition: A Case Study on Hafnium Oxide Process Optimization

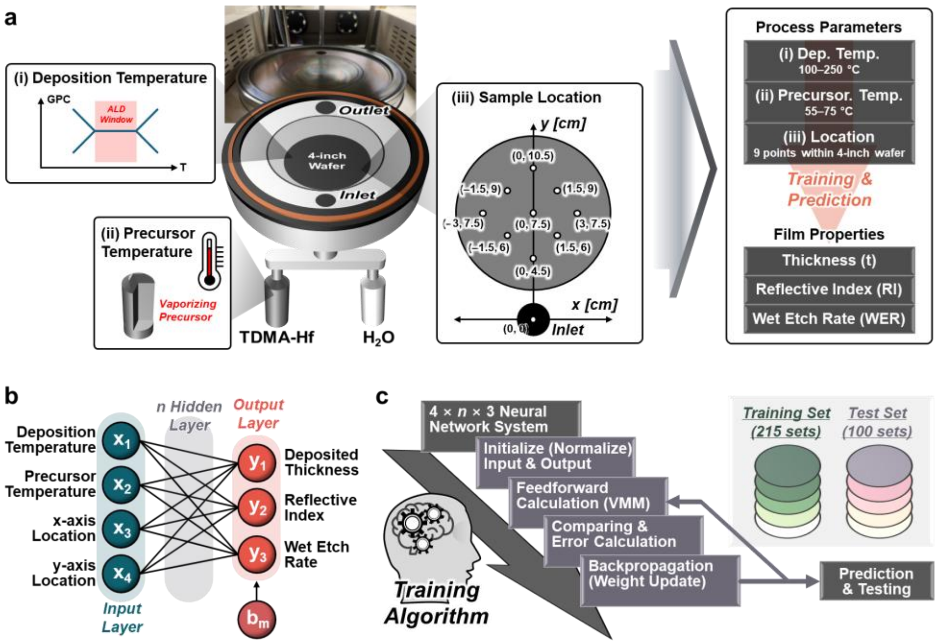

Fig. 1. Schematics of the ALD process and deep neural network (DNN) framework for HfO_x film deposition. (a) ALD process parameters: (i) deposition temperature, (ii) precursor temperature for TDMA-Hf, and (iii) sample location coordinates on a 4-inch wafer. The process parameters and film properties of interest are displayed on the right. (b) DNN architecture with 4 input neurons representing ALD parameters and 3 output neurons for film properties (deposited thickness (T_{ox}), reflective index (RI), and wet etch rate (WER). (c) Training and testing algorithm for the multi-layer NN system, utilizing 215 datasets for training and 100 datasets for testing.

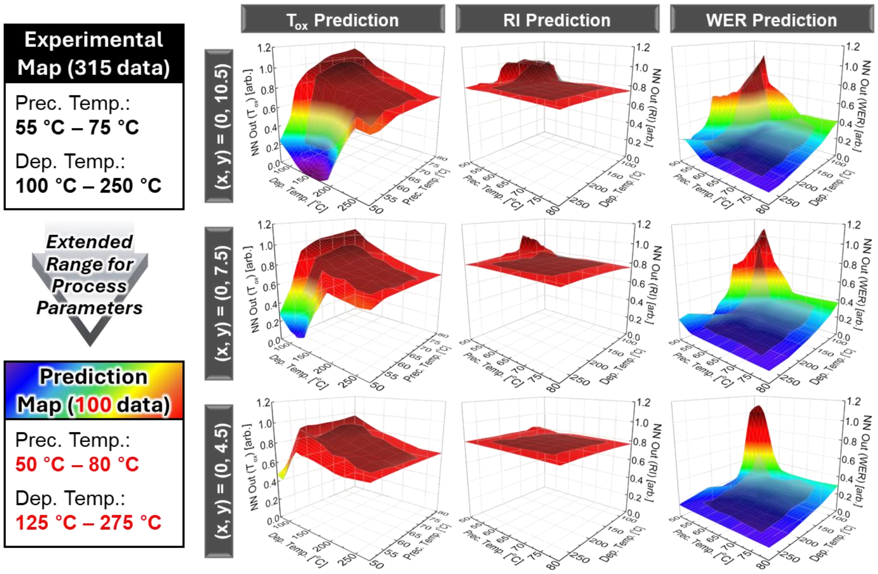

Fig. 2. 3D surface plots showing experimental and prediction maps for three film properties: T_{ox}, RI, and WER. The plots are arranged in three rows representing different sample locations (x, y) = (0, 10.5), (0, 7.5), and (0, 4.5). Each column corresponds to a specific property prediction (T_{ox}, RI, WER). The experimental map (black-colored plots) covers precursor temperatures of 55–75 °C and deposition temperatures of 100–250 °C. The prediction maps (colored plots) extend these ranges to 50–80 °C for precursor temperature and 125–275 °C for deposition temperature, demonstrating the capability of the ML-based model to predict film properties over an extended range of process parameters.