Machine Learning for Accelerating Atomic Layer Deposition Process Optimization

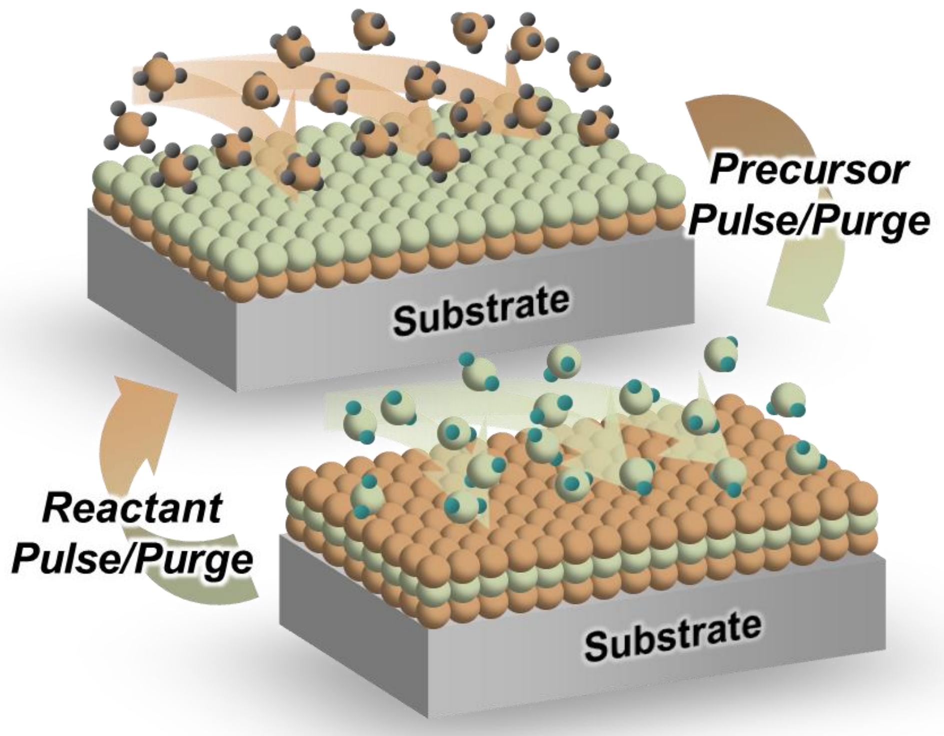
Minjong Lee, Doo San Kim, Dushyant M. Narayan, and Jiyoung Kim*

[1]*The University of Texas at Dallas, TX, USA*
* *jiyoung.kim@utdallas.edu*

Background and motivation

Atomic layer deposition (ALD)

Atomic Layer Deposition (ALD)



Angstrom (Å)-scaled controllability

- ALD process is based on **Saturation** processes
  => **Wide process windows**

  => Relatively **long process** time
  => low throughputs
  => **Excess use** of precursors and reactants

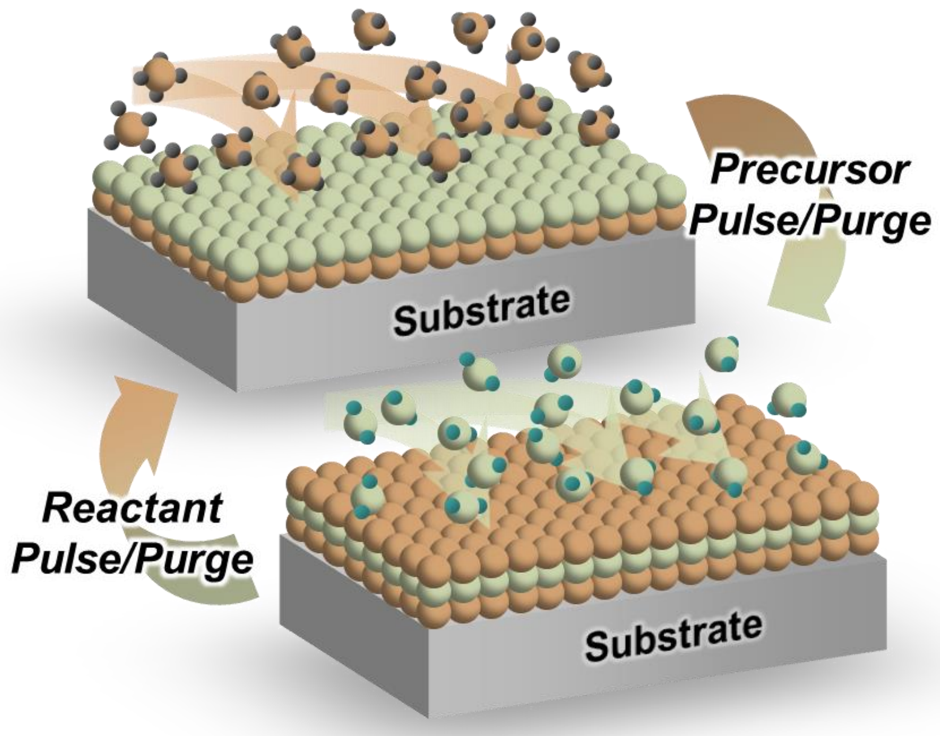
- If non-ideal ALD process is performed, then the thin film quality would be pretty different from what you expect (potentially not desirable)

- ML for Autonomous ALD Process

Background and motivation

Atomic layer deposition (ALD)

- **Atomic Layer Deposition (ALD)**



Angstrom (Å)-scaled controllability

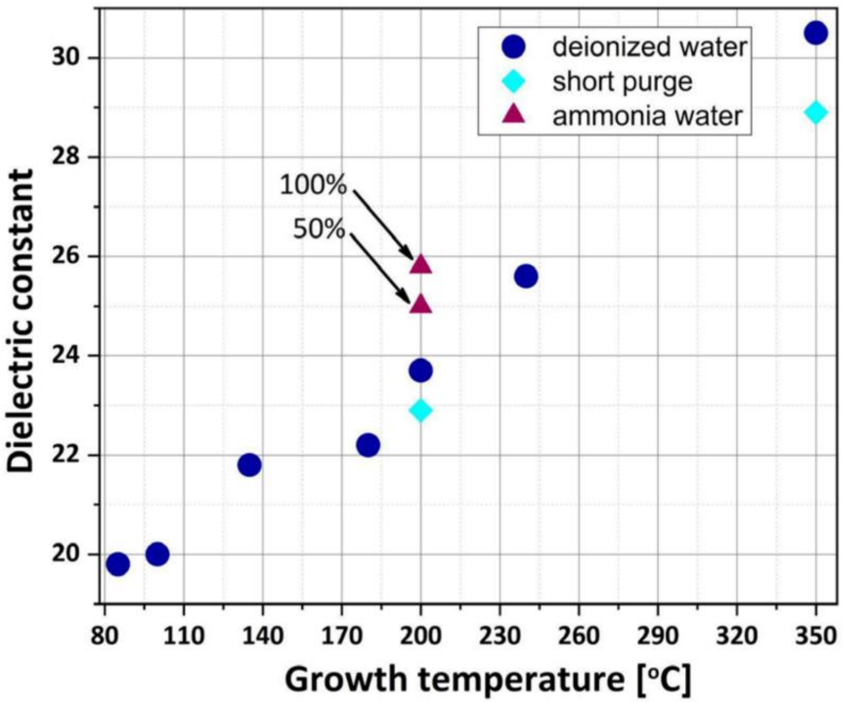
ALD Process Parameters	
Precursor Pulse Time	*Sample Locations*
Precursor Purge Time	*Reaction Chamber*
Reactant Pulse Time	*Plasma or Thermal*
Reactant Purge Time	*Purging Gas*
Cycle Number	*Flow Tube Reaction*
Deposition Temperature	*Pumping Capacity*
Precursor Temperature	*Working Pressure*
Precursor Sources	*Gas Line Length*
Reactant Sources	*Reaction Substrate*

Background and motivation

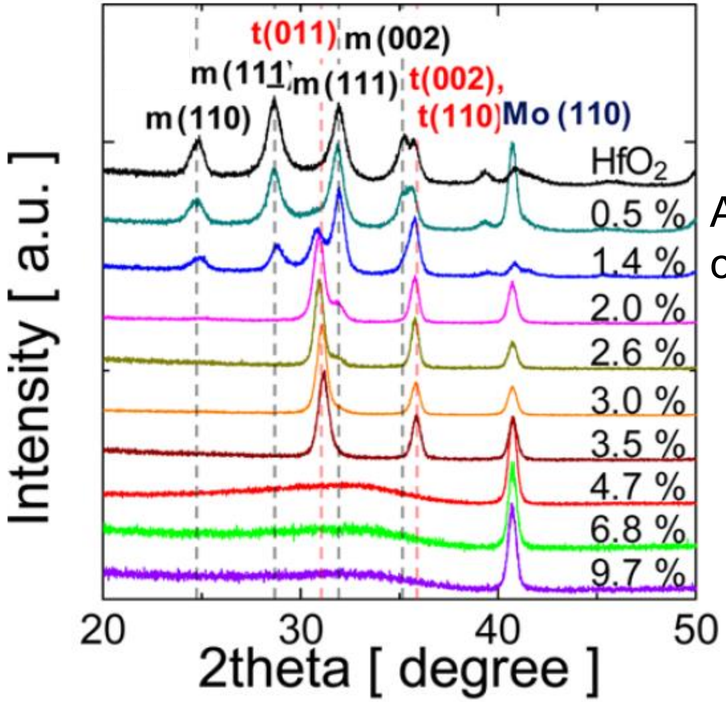
Process optimization (Case of HfO_2)

Process Optimization for high-quality film & high-performance device

[1]



[2]



Al doping concentration

The deposition profile in ALD directly influences film quality and electrical performance

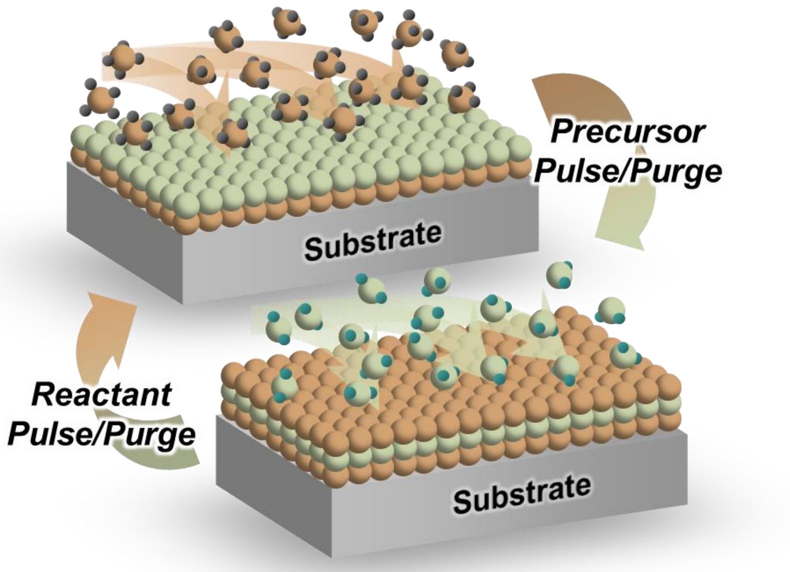
[1] S. Gieraltowska et al., *Materials* **16**, 4077 (2023). [2] Y. W. Yoo et al., *ACS Appl. Mater. Interfaces* **6**, 22474–22482 (2014).

Background and motivation

Emerging 3D structure

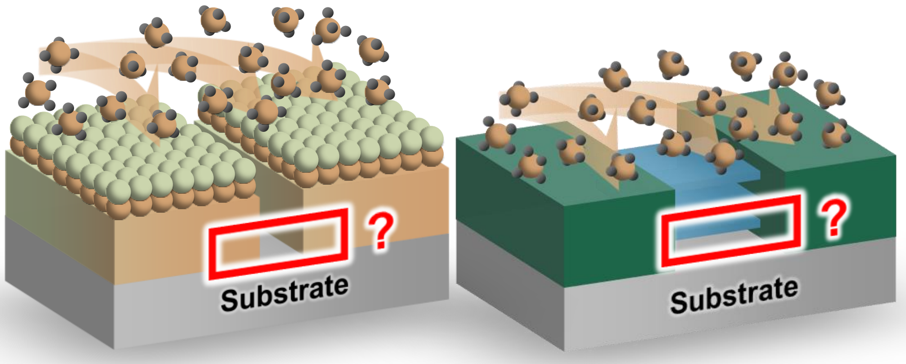
Complex Process Steps of Current ALD Technologies

Conventional
2D planar structure



Simply growing thin film
on 2D planar structure

More complex 3D structures
have been emerged



Monitoring 3D structures
is even more complex to be predicted

Deeper understanding
and analysis is necessary

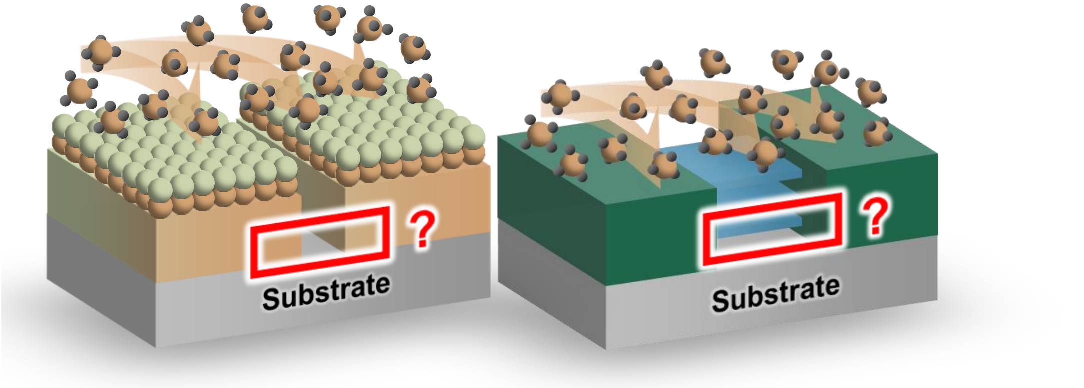
Background and motivation

Machine learning (ML) for ALD

Many ALD parameters must be optimized to achieve **high-quality films** and, ultimately, **high performance device**

ALD Process Parameters	
Precursor Pulse Time	*Sample Locations*
Precursor Purge Time	*Reaction Chamber*
Reactant Pulse Time	*Plasma or Thermal*
Reactant Purge Time	*Purging Gas*
Cycle Number	*Flow Tube Reaction*
Deposition Temperature	*Pumping Capacity*
Precursor Temperature	*Working Pressure*
Precursor Sources	*Gas Line Length*
Reactant Sources	*Reaction Substrate*

In **3D structures**, it is **difficult to know what occurs deep inside** the features, highlighting the need for deeper structural analysis and understanding.



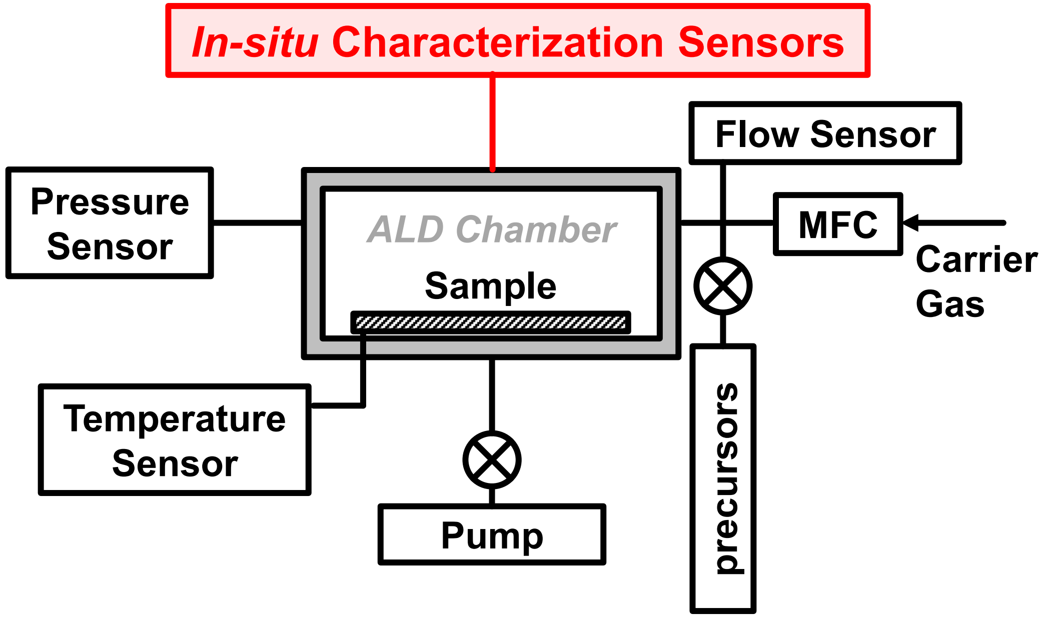
***Machine learning (ML)* offers a powerful tool to interpret ALD behavior and extract insights from complex process data**

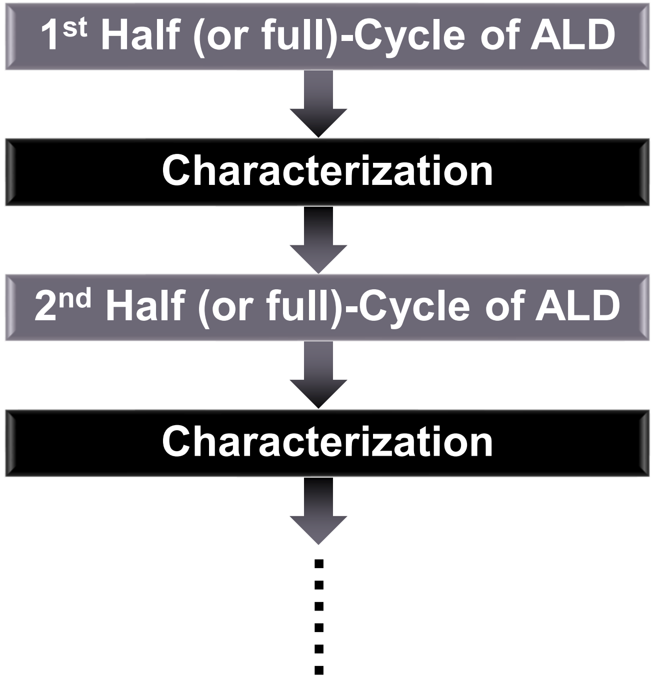
Background and motivation

Machine learning (ML) for ALD

In-situ ALD process

To achieve **"self-feedback ML-driven ALD system,"** the ***in-situ* monitoring** is helpful





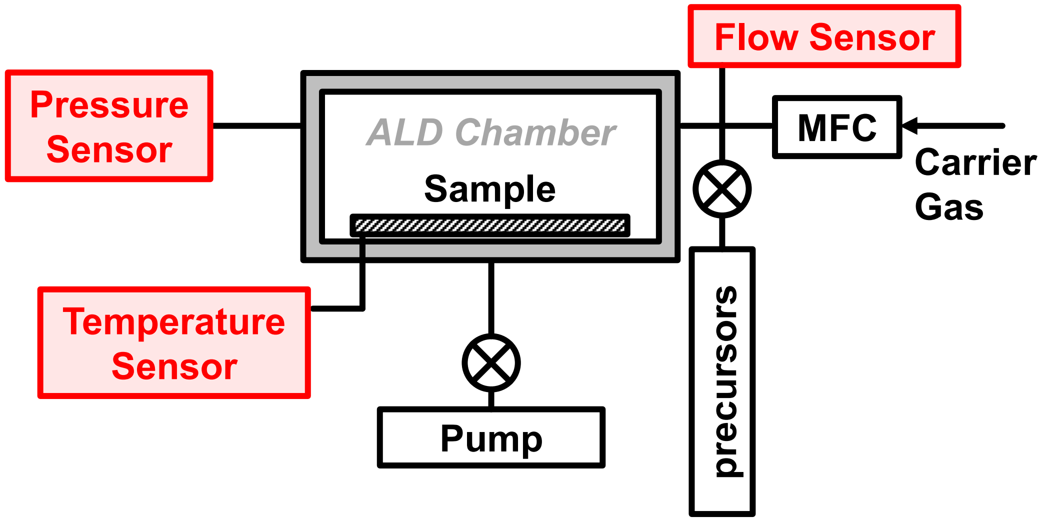
Economically & Efficiently unfeasible!

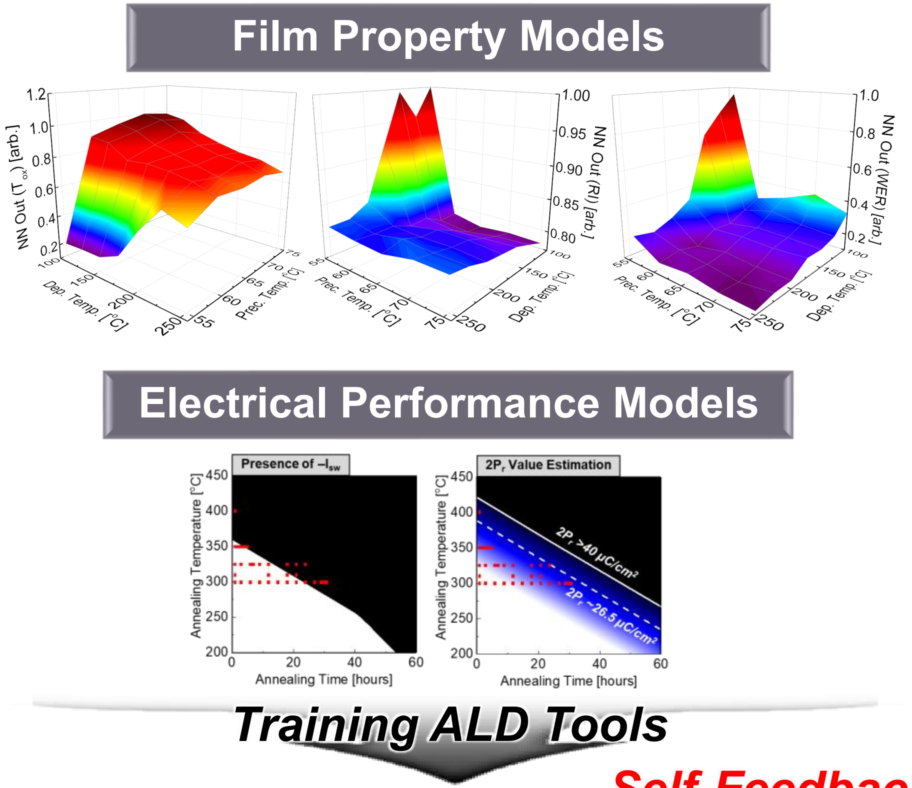
Our Approach

Proof-of-concepts for ML-driven ALD processes

- **“Pipeline” framework for autonomous ALD tool**

Self-feedback ML-driven ALD system, **by using the conventional process sensors** (e.g., pressure, temp.)



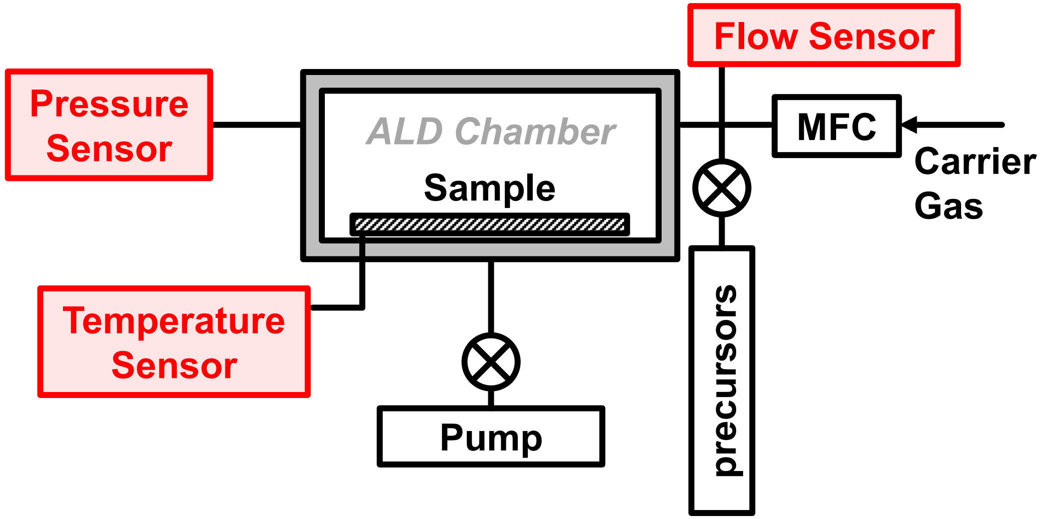


Our Approach

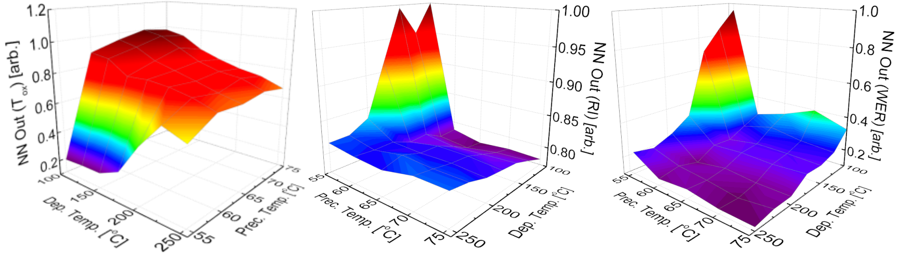
Proof-of-concepts for ML-driven ALD processes

- **"Pipeline" framework for autonomous ALD tool**

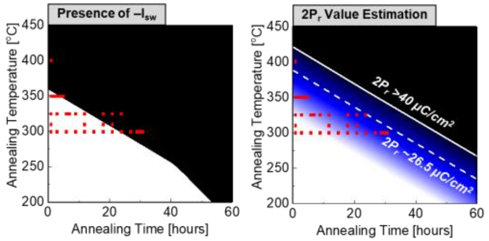
Self-feedback ML-driven ALD system, **by using the conventional process sensors** (e.g., pressure, temp.)



Film Property Models



Electrical Performance Models



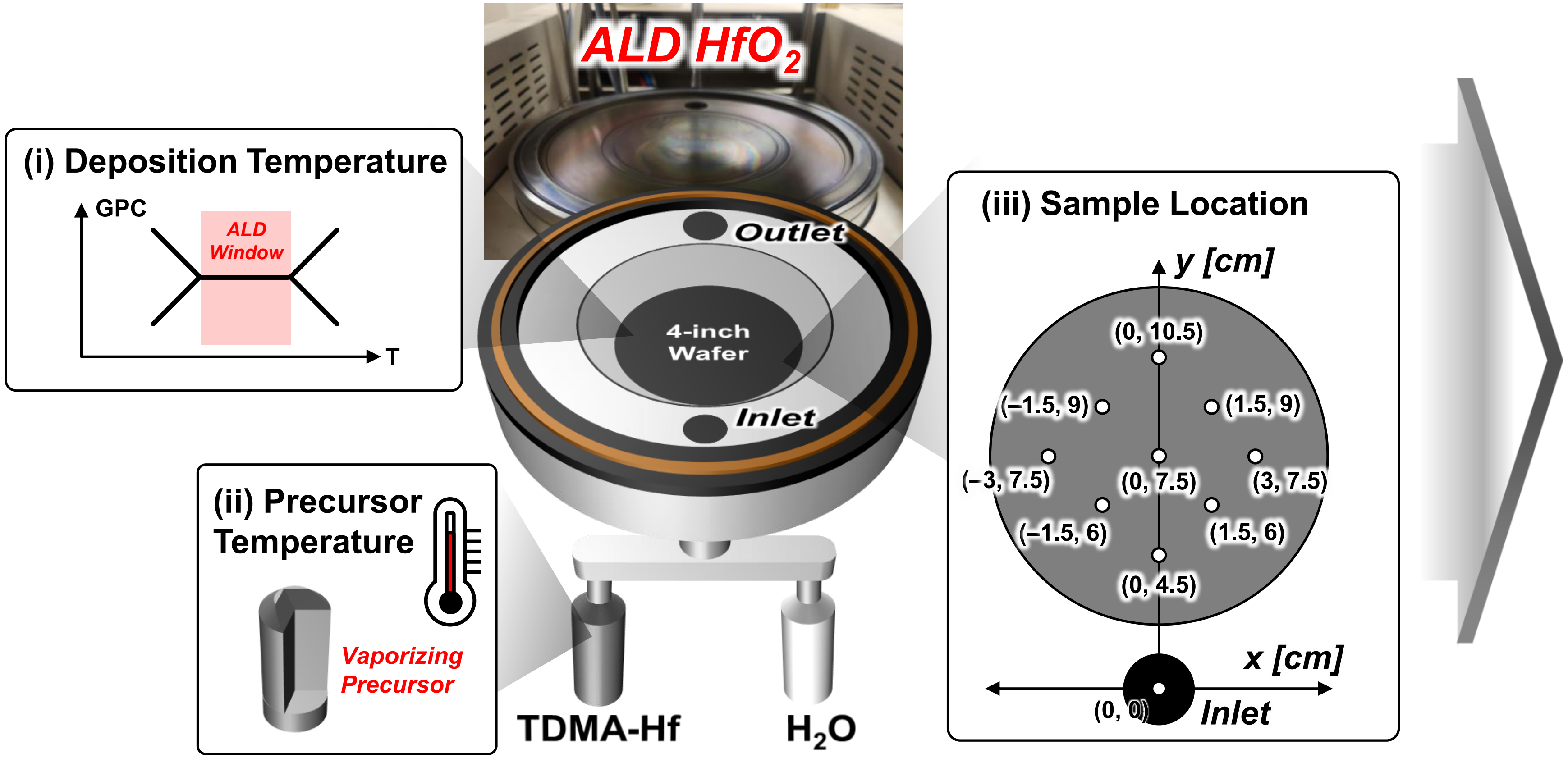
Training ALD Tools

Self-Feedback During ALD

ML-Driven ALD Processes

Case studies of hafnium oxide growth on silicon substrate

Process variations and film properties of interest



Process Parameters

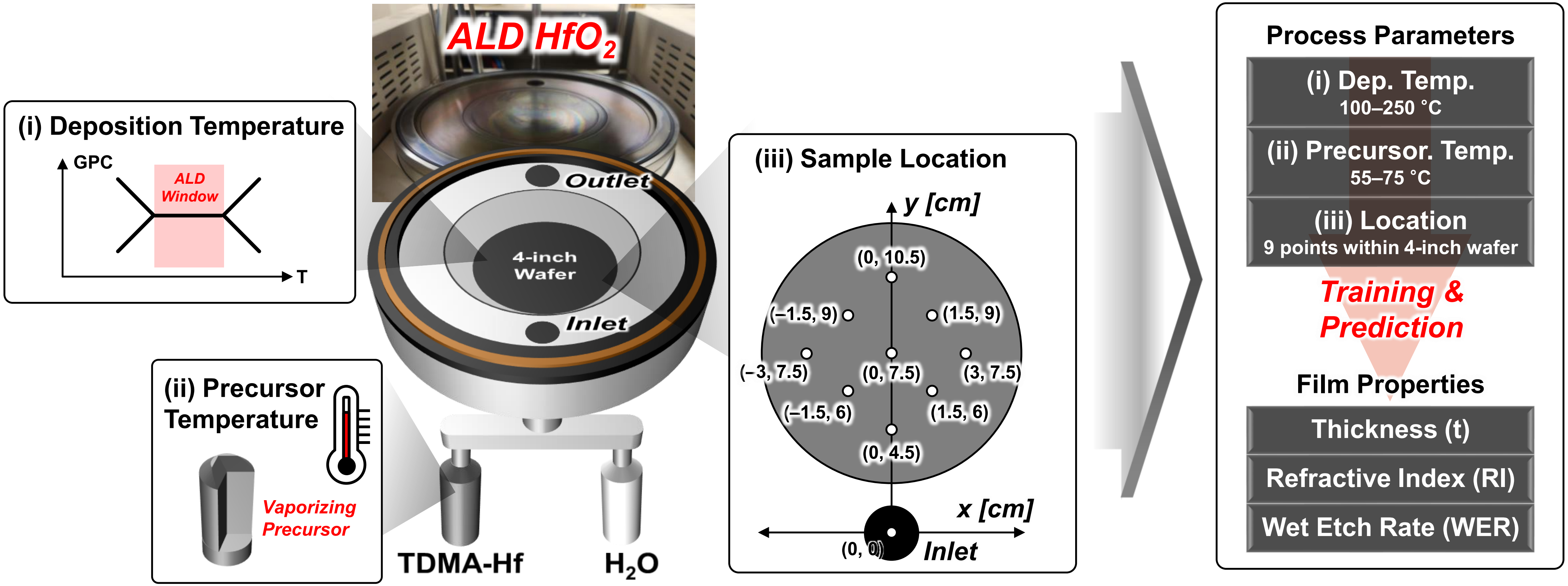
(i) Dep. Temp. 100–250 °C
(ii) Precursor. Temp. 55–75 °C
(iii) Location 9 points within 4-inch wafer

Three ALD parameters were controlled:
Deposition temp., precursor temp., sample location

ML-Driven ALD Processes

Case studies of hafnium oxide growth on silicon substrate

Process variations and film properties of interest

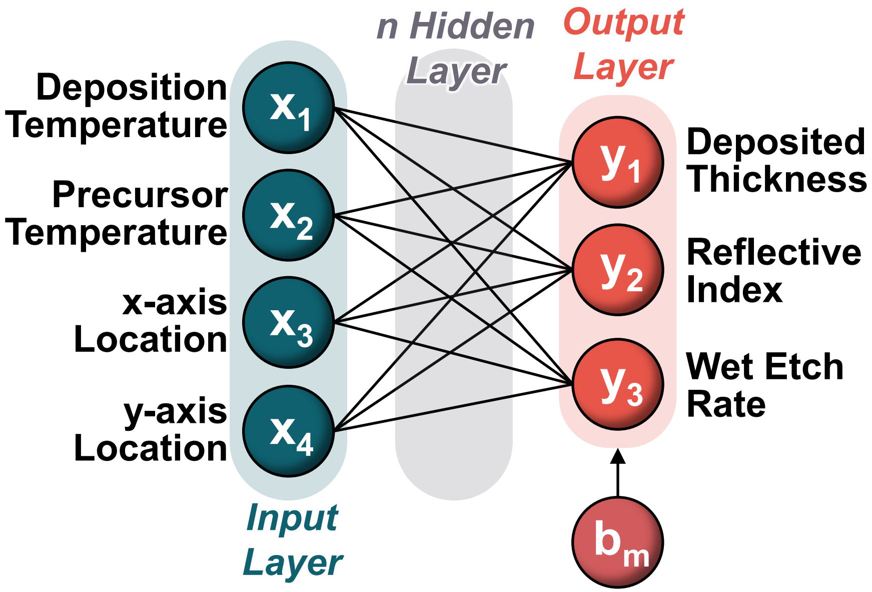


Three ALD parameters were controlled:
Deposition temp., precursor temp., sample location

ML-Driven ALD Processes

ML-driven ALD process workflow

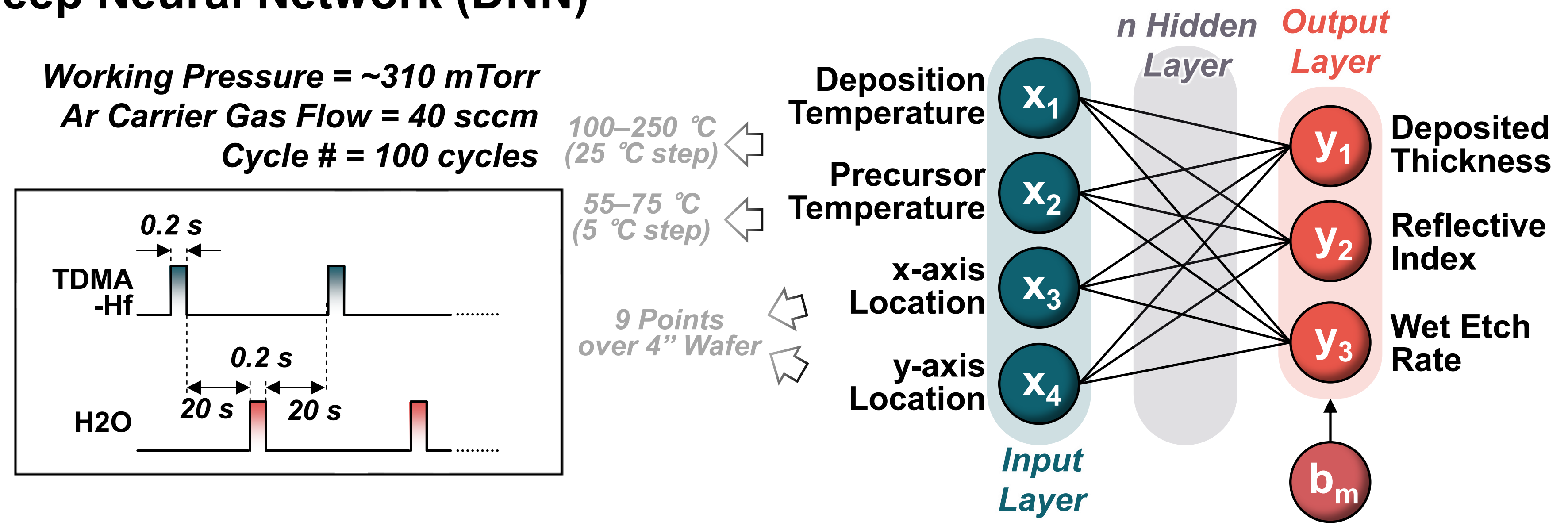
- Deep Neural Network (DNN)



ML-Driven ALD Processes

ML-driven ALD process workflow

Deep Neural Network (DNN)

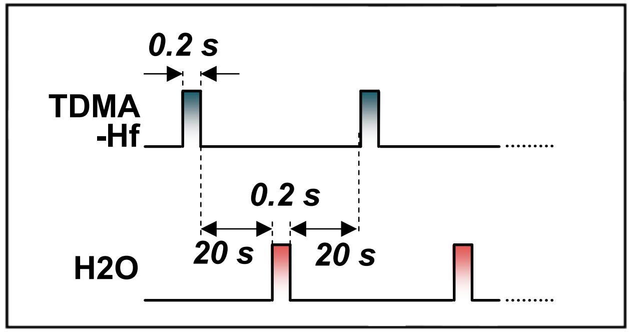


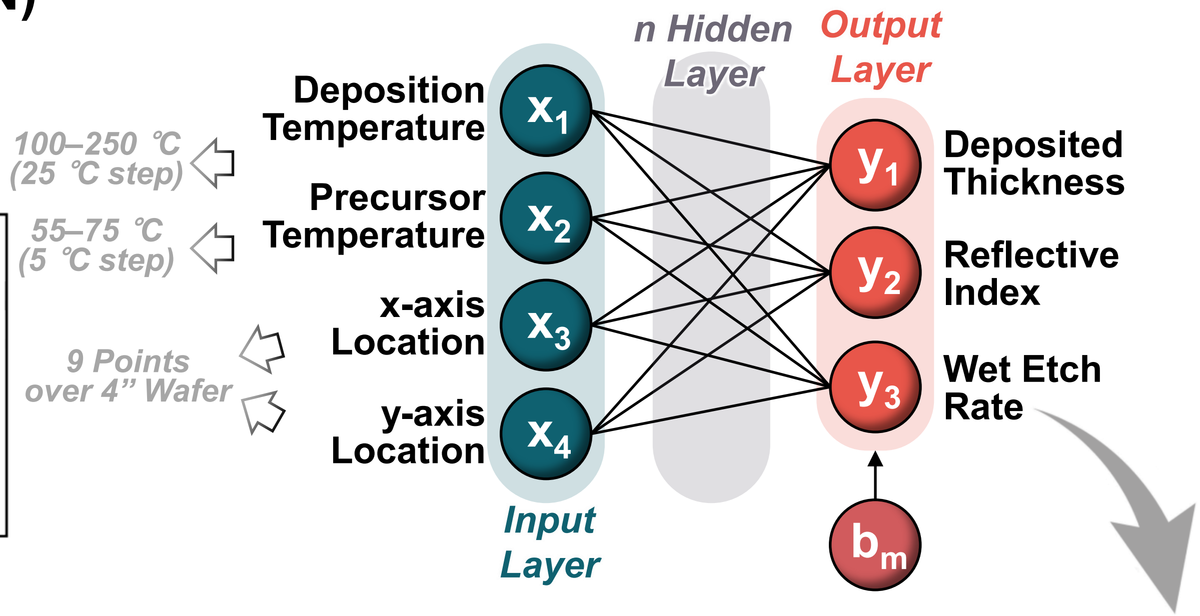
ML-Driven ALD Processes

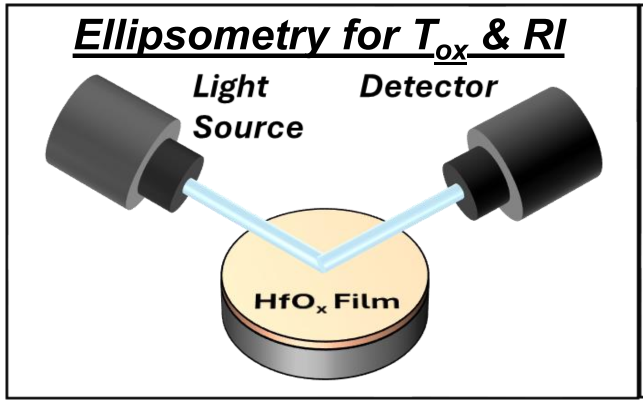
ML-driven ALD process workflow

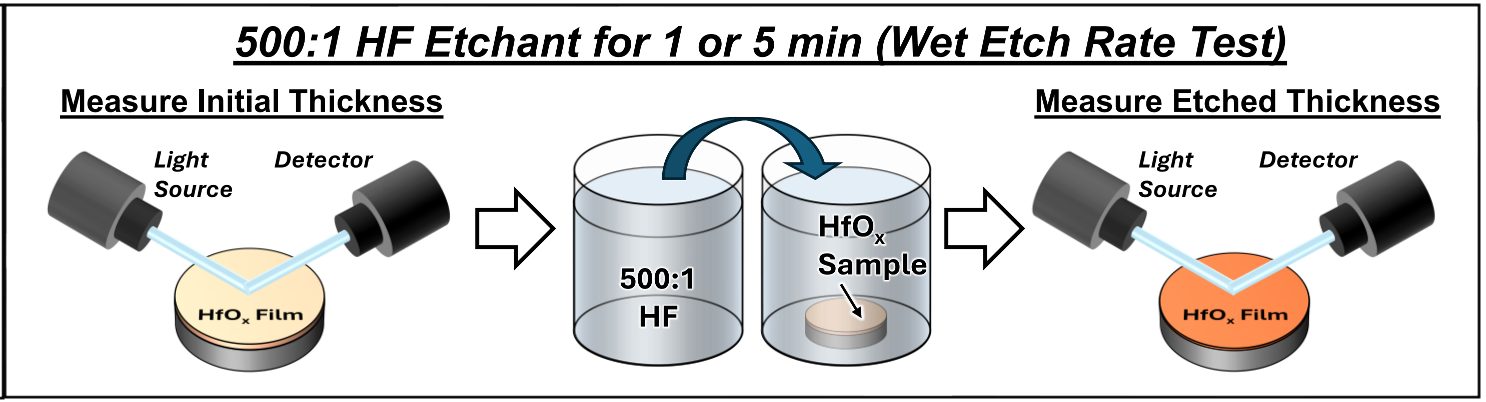
Deep Neural Network (DNN)

Working Pressure = ~310 mTorr
Ar Carrier Gas Flow = 40 sccm
Cycle # = 100 cycles





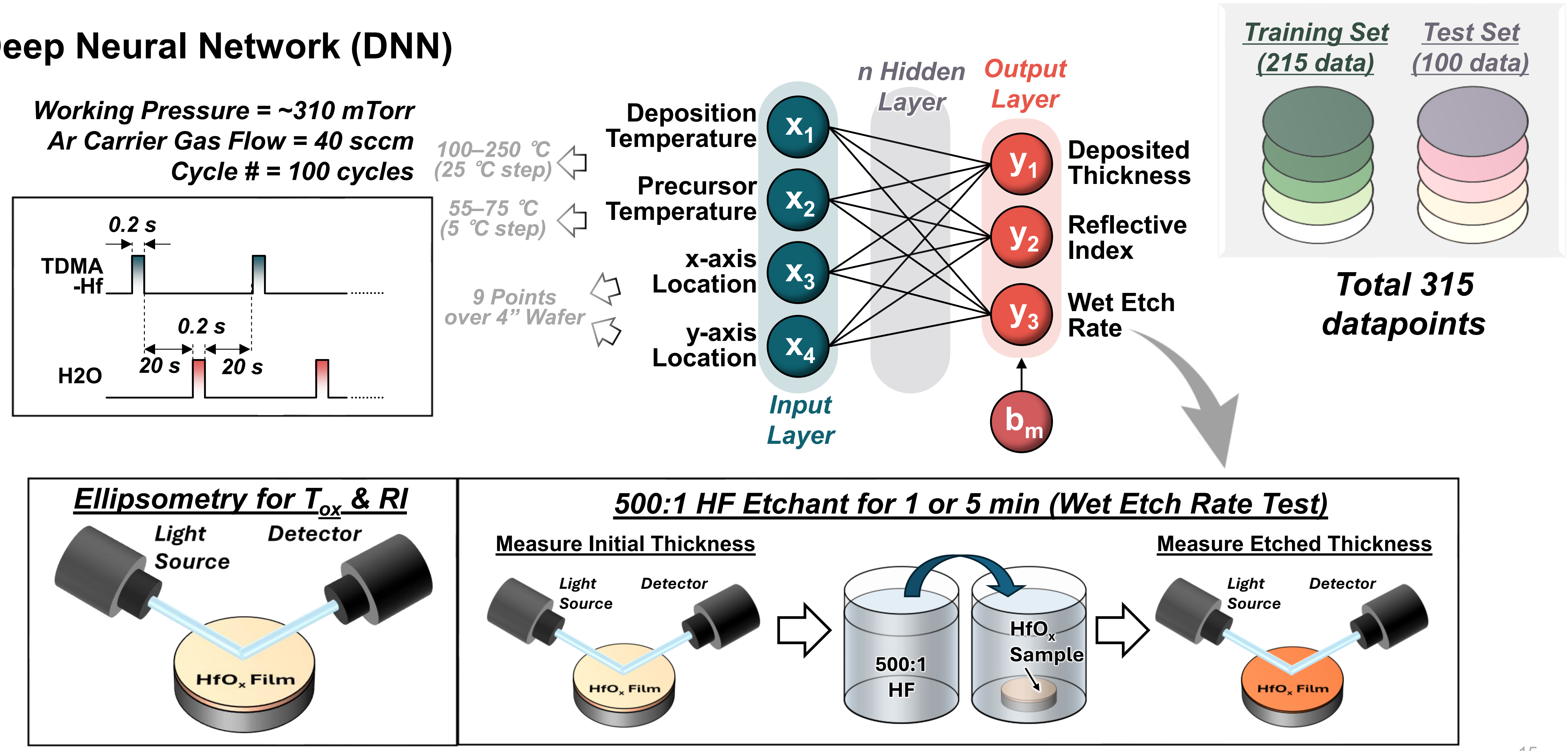




ML-Driven ALD Processes

ML-driven ALD process workflow

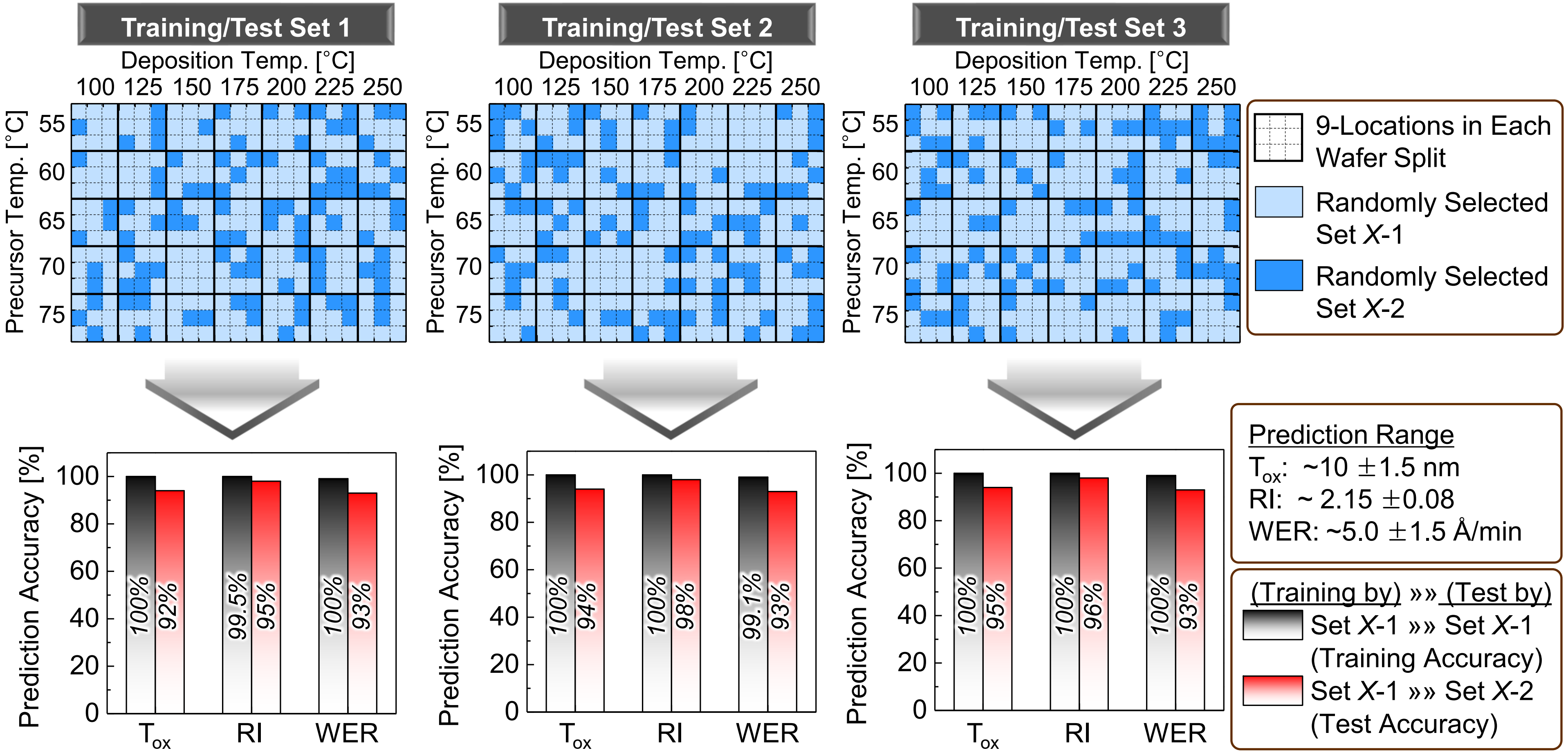
Deep Neural Network (DNN)



ML-Driven ALD Processes

Predictive work using ML

Prediction accuracy

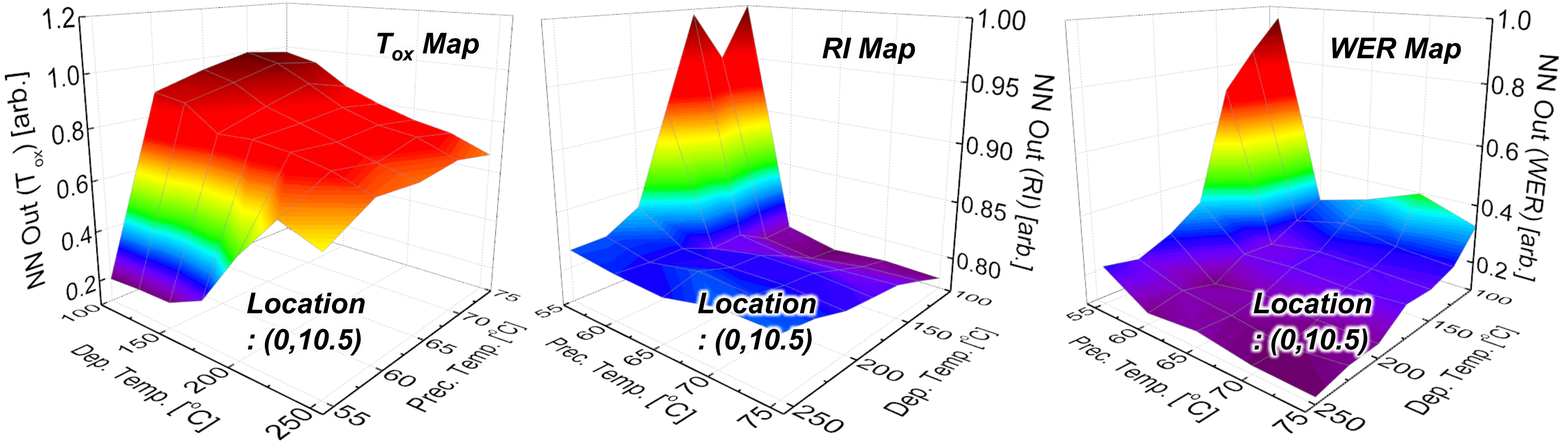


ML-Driven ALD Processes

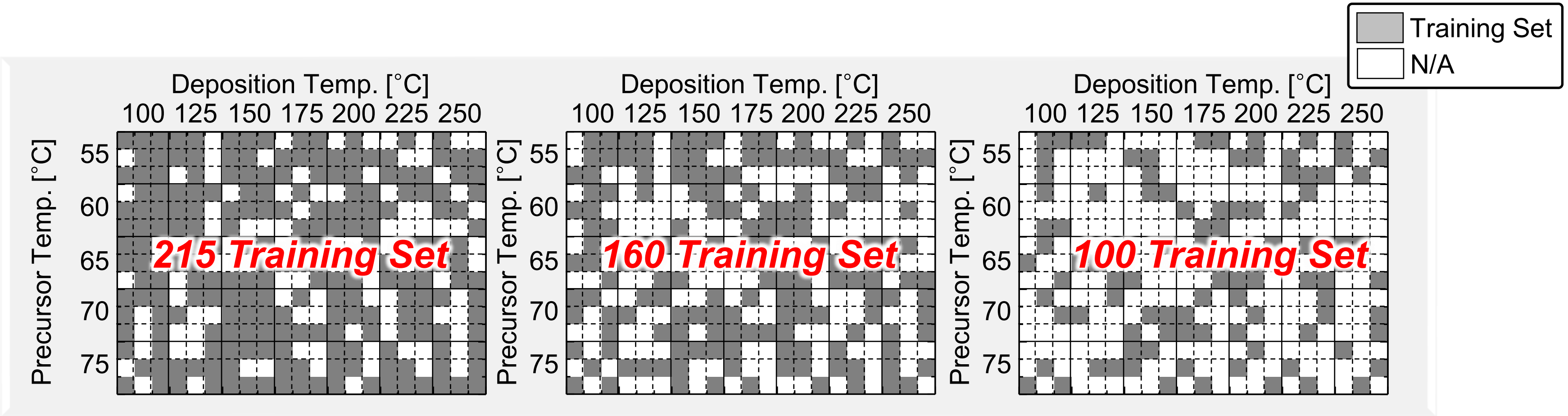
ALD prediction maps

Prediction maps

Physical Space
Experimental Map



Virtual Space
Prediction Map



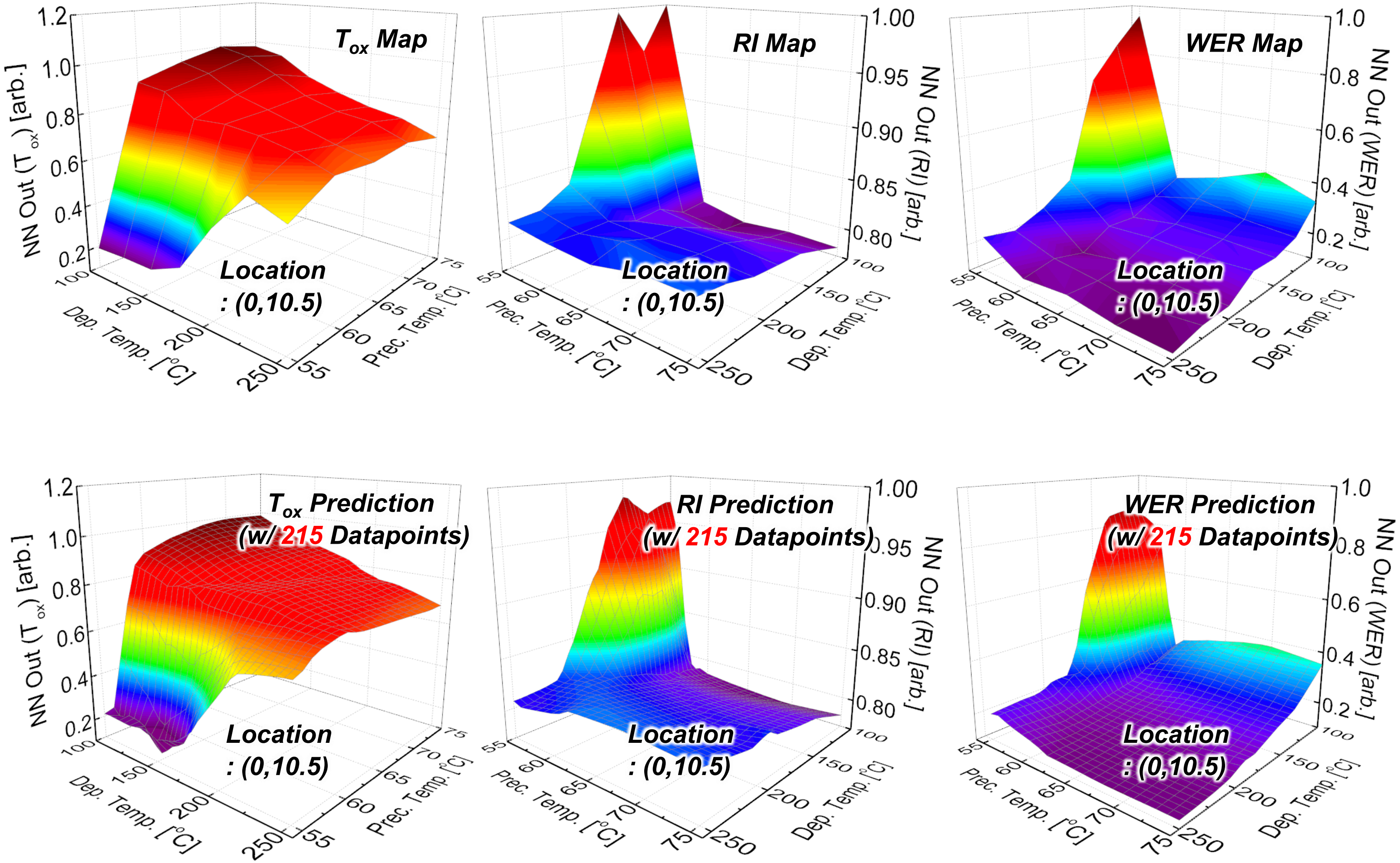
ML-Driven ALD Processes

ALD prediction maps w/ 215 datapoints

Prediction maps

Physical Space

Experimental Map



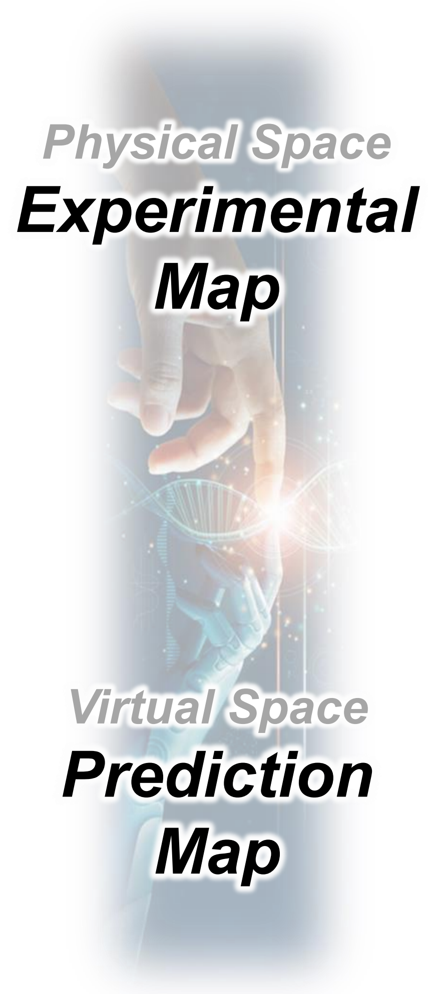
Virtual Space

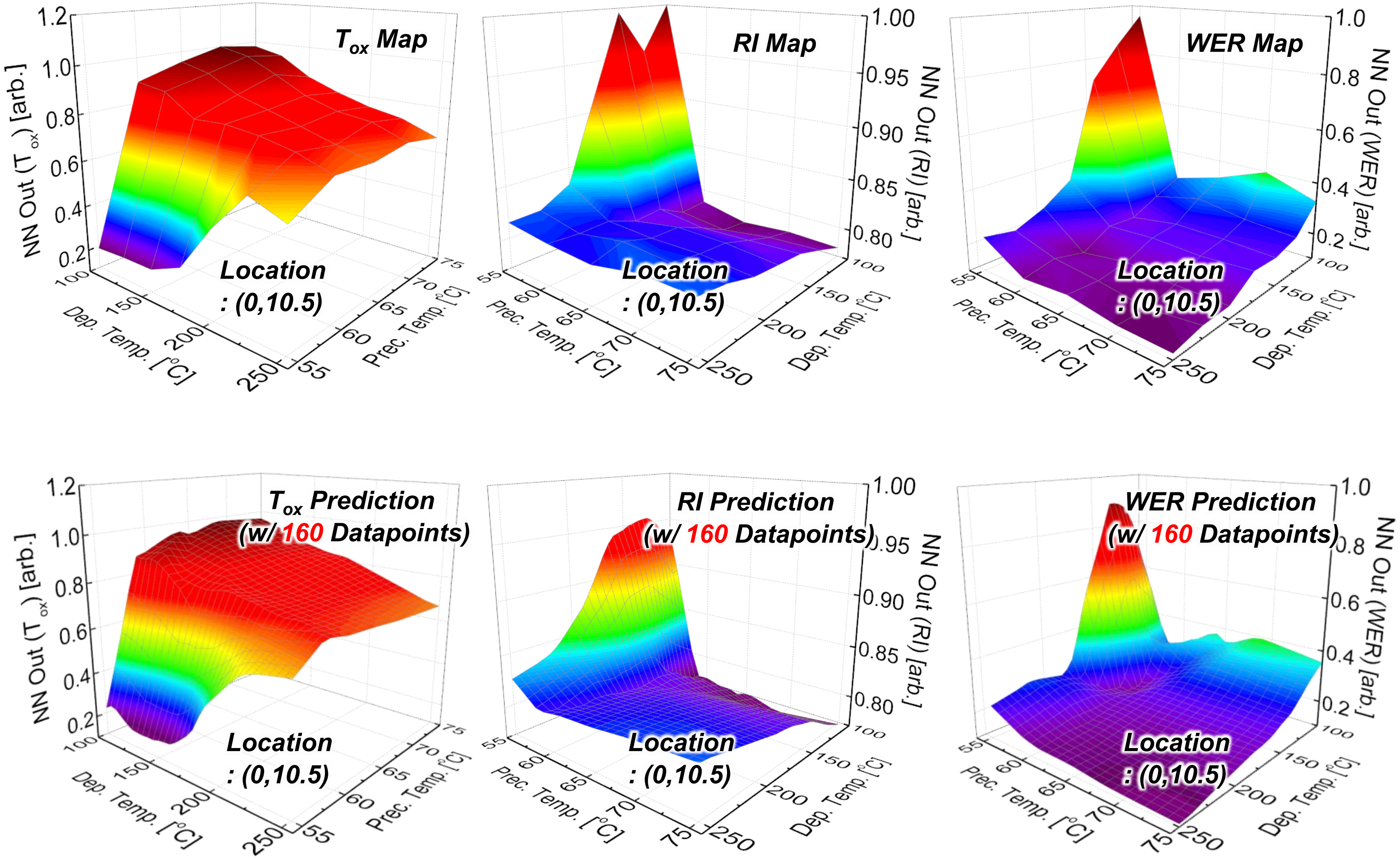
Prediction Map

ML-Driven ALD Processes

ALD prediction maps w/ 160 datapoints

Prediction maps





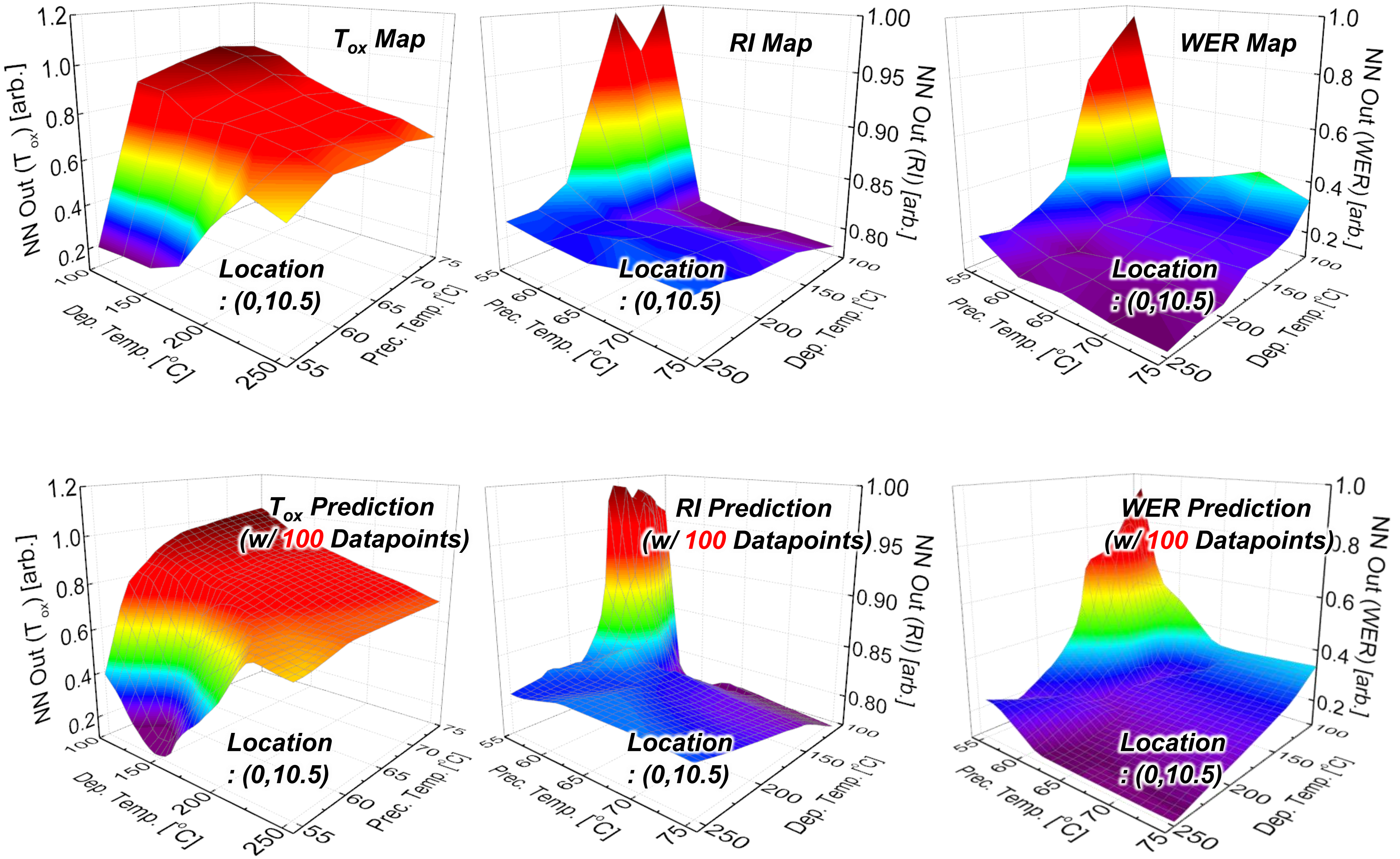
ML-Driven ALD Processes

ALD prediction maps w/ 100 datapoints

Prediction maps

Physical Space
Experimental Map

Virtual Space
Prediction Map



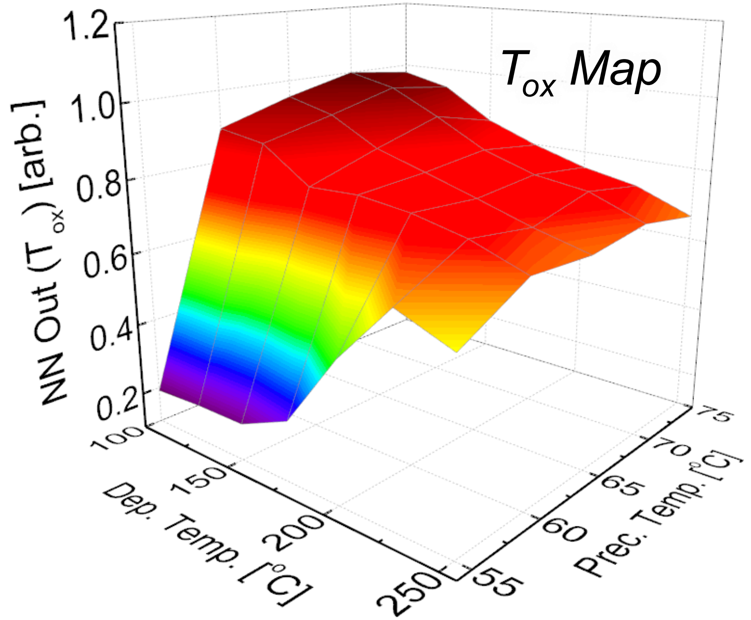
ML-Driven ALD Processes

ALD prediction maps

Prediction maps

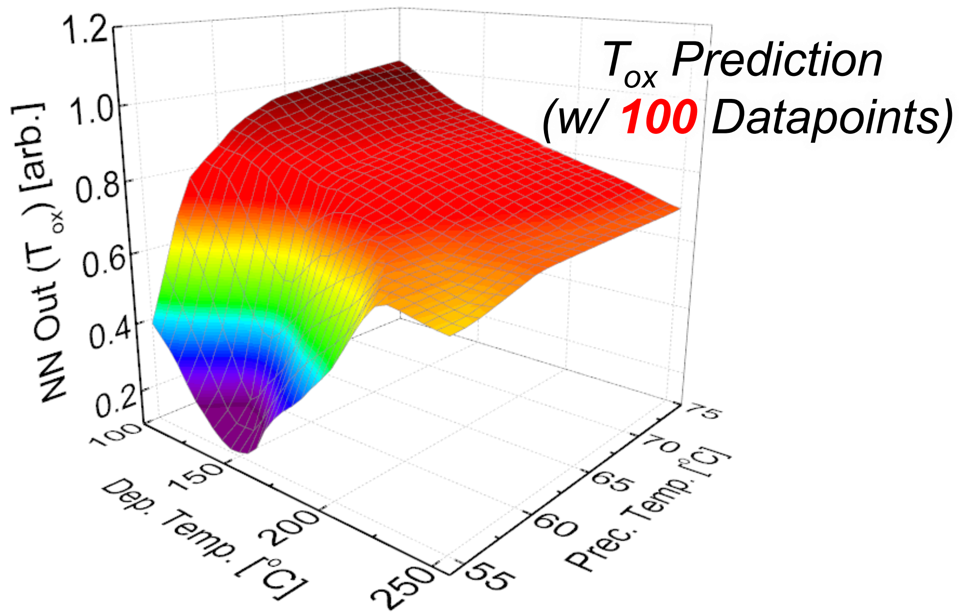
Physical Space

Experimental Map



Virtual Space

Prediction Map



The prediction map successfully captures the growth trend as a function of deposition and precursor temperatures

ML-Driven ALD Processes

ALD prediction maps

- **Extended prediction maps (ML-based trained map w/ 100 datapoints)**

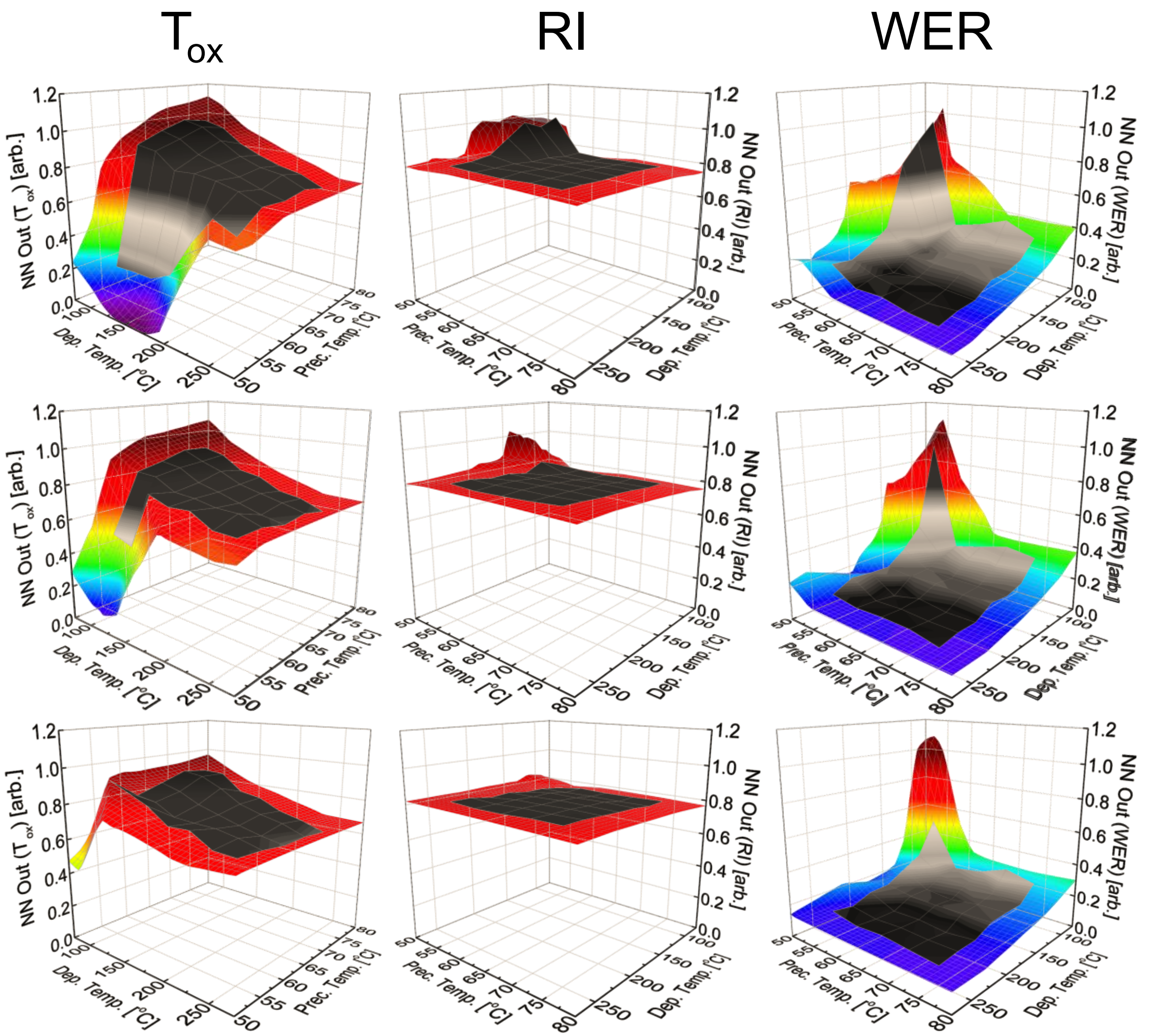
Precursor Temperature:
55 °C – 75 °C
Deposition Temperature:
100 °C – 250 °C

Precursor Temperature:
50 °C – 80 °C
Deposition Temperature:
75 °C – 275 °C

(x, y) = (0, 10.5)

(x, y) = (0, 7.5)

(x, y) = (0, 4.5)



ML-Driven ALD Processes

ALD prediction maps

- **Extended prediction maps (ML-based trained map w/ 100 datapoints)**

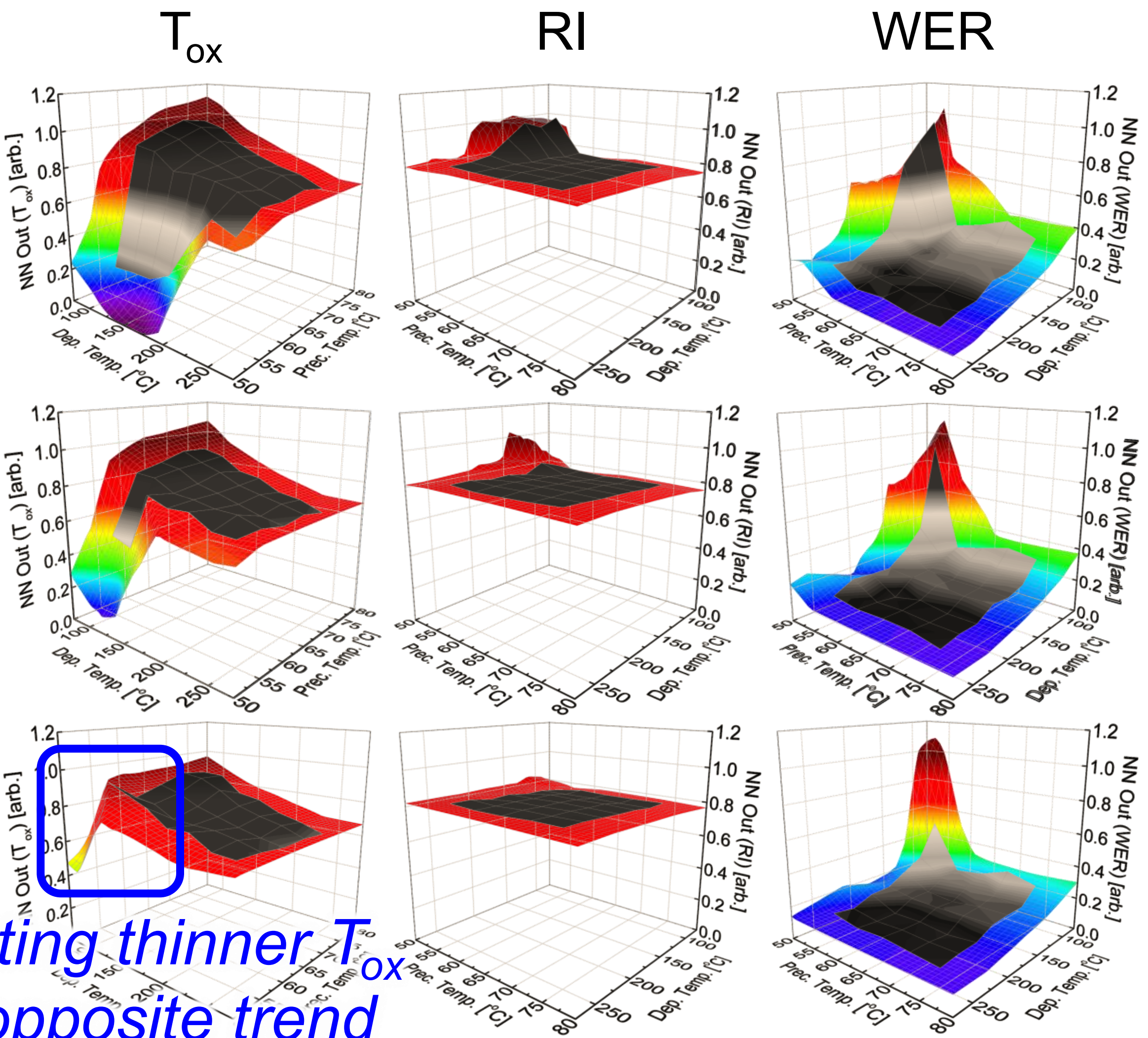
Precursor Temperature:
55 °C – 75 °C
Deposition Temperature:
100 °C – 250 °C

Precursor Temperature:
50 °C – 80 °C
Deposition Temperature:
75 °C – 275 °C

(x, y) = (0, 10.5)

(x, y) = (0, 7.5)

(x, y) = (0, 4.5)



Predicting thinner T_{ox} with opposite trend

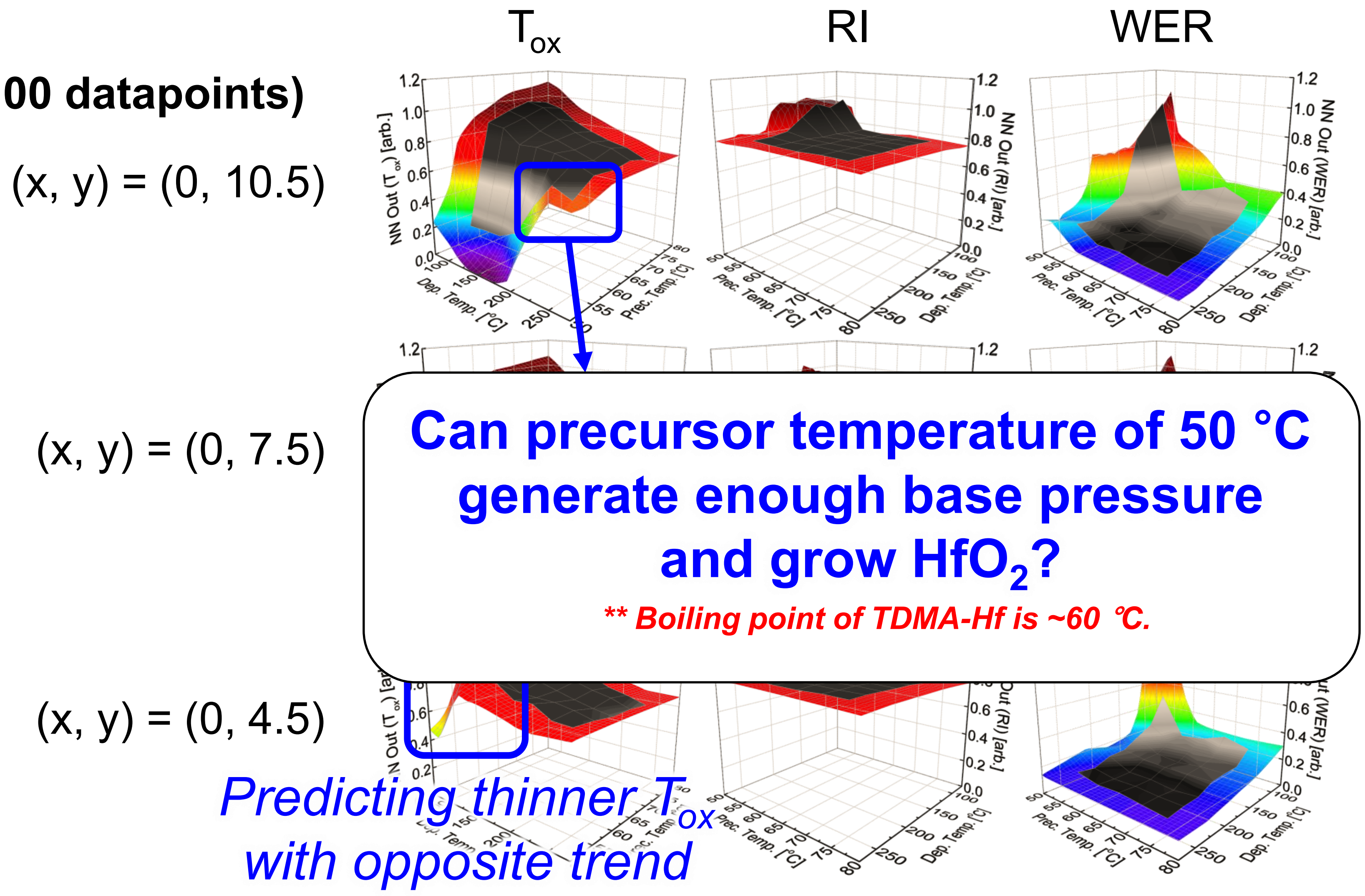
ML-Driven ALD Processes

ALD prediction maps

Extended prediction maps (ML-based trained map w/ 100 datapoints)

Precursor Temperature:
55 °C – 75 °C
Deposition Temperature:
100 °C – 250 °C

Precursor Temperature:
50 °C – 80 °C
Deposition Temperature:
75 °C – 275 °C



Can precursor temperature of 50 °C generate enough base pressure and grow HfO_2?

*** Boiling point of TDMA-Hf is ~60 ℃.*

Predicting thinner T_{ox} with opposite trend

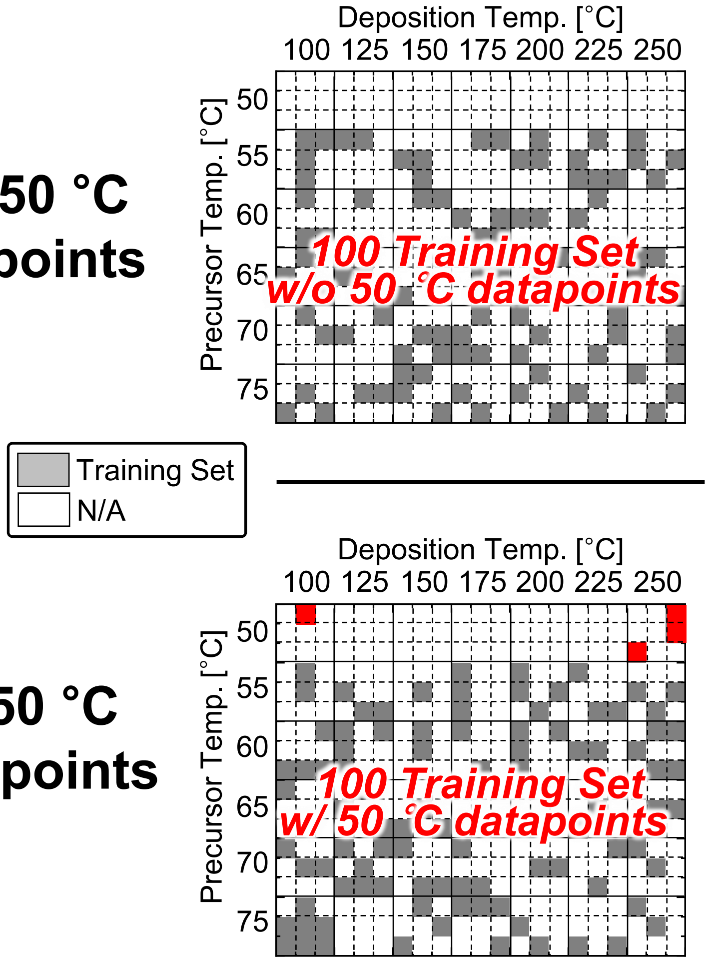
ML-Driven ALD Processes

ALD prediction maps

- **Include 50 °C training data**

w/o 50 °C datapoints

w 50 °C datapoints

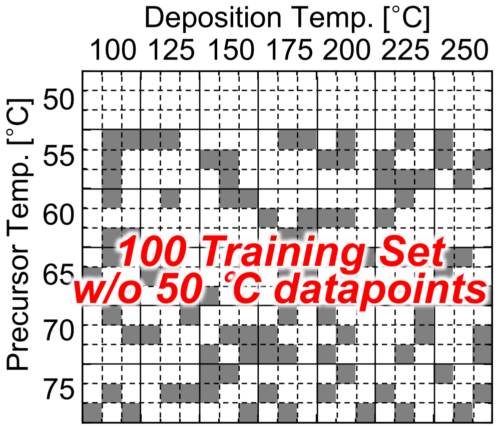


ML-Driven ALD Processes

ALD prediction maps

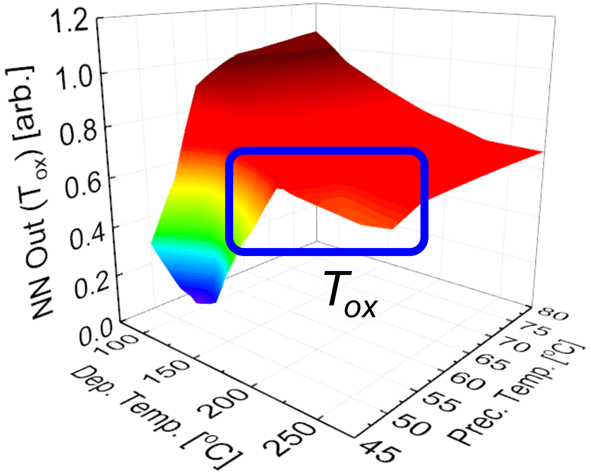
- **Include 50 °C training data**

w/o 50 °C datapoints



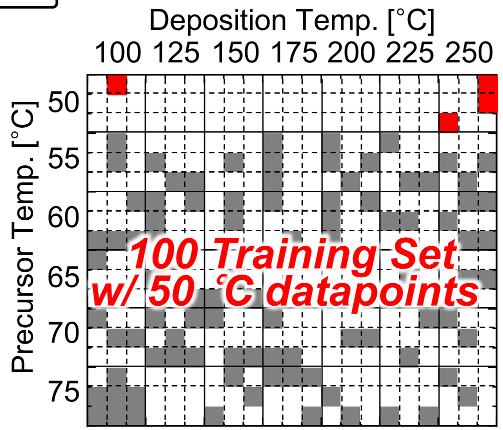
Precursor Temperature:
50 °C – 80 °C

Deposition Temperature:
75 °C – 275 °C



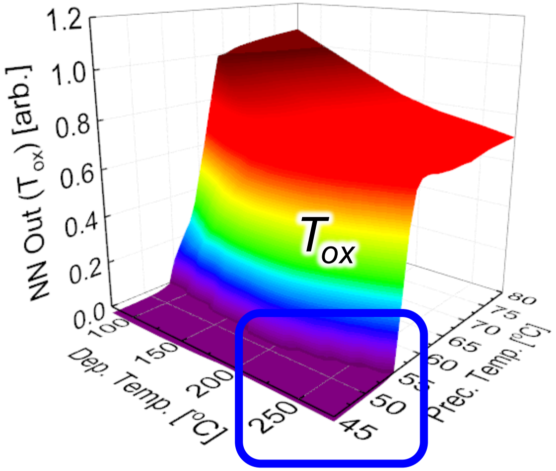
Training Set
N/A

w 50 °C datapoints



Precursor Temperature:
45 °C – 80 °C

Deposition Temperature:
75 °C – 275 °C



Summary

- ❑ **Machine learning (ML) can offer a powerful tool to interpret ALD behavior and extract insights from complex process data**

✓ Many ALD parameters needed to be controlled for process optimization

✓ Deeper understanding for 3D structures

✓ “Pipeline research” on how we can apply machine learning to ALD process efficiently

- ❑ **ML-driven ALD processes using DNN systems**

✓ Apply ML to the ALD process through the use of process parameters as inputs and prediction of film properties as outputs

✓ Assess the required number of training datapoints

✓ Demonstrate the advantages of machine learning, particularly in enabling broader exploration of the process parameter space

✓ Including poor or failed results in training data is critical for improving the accuracy of ML predictions

Perspectives

- ❑ ***In-operando* Auto-Reprogramming Process based on ML Predictions**

- ✓ In-operando measurements big-data sets enable to predict the film qualities/properties using ML
- ✓ Training the tool that can modify process parameters to obtain the expected target results *during the process*
- ✓ Eventually, add 3D process and characteristics capabilities for advanced semiconductor processing

- ❑ **Even Further Predictions on Device Electrical/Reliability Characteristics**

- ❑ **Autonomous ALD process to enhance manufacturing capabilities and the thin film qualities**

Thank you

Questions?
Email to
Jiyoung.Kim@utdallas.edu