Oxide Etch Rate Prediction under Varying O_2 using Stepwise Forward Selection of Principal Components

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1. 연구 배경 및 목적 (INTRODUCTION)

- **Challenges in Process Control**

Delay in physical metrology limits immediate Run-to-Run (R2R) control.

- **Objective**

Construct a sensor-based Virtual Metrology (VM) model to predict SiO_2 etch rate in real-time under O_2 gas variations causing severe multicollinearity, establishing a decorrelated variable pipeline through chemical/physical insight.

2. 데이터 파이프라인 (DATA PIPELINE)

Raw Data (OES, VI)

Feature Filtering

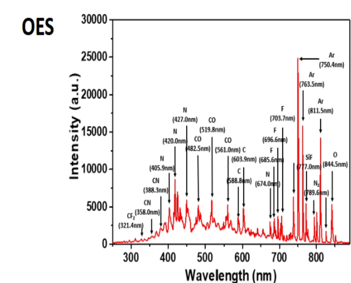
OES variables (12)

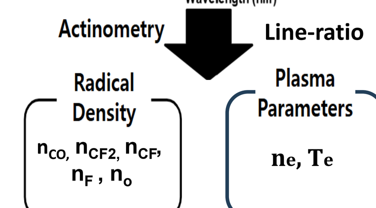
- **Actinometry ($n_F \propto I_F/I_{Ar}$)**
  - Tracks relative radical densities -F (703.57, 686.60nm), O (777.03, 700.65nm), CF_2 (251.86, 262.80nm), CF (258.12, 724.06nm), CO (645.4, 644.44nm) against an Ar (750.49nm) reference to counter gas volatility.
- **Ar Line-ratio (n_e, T_e)**
  - Selects 706.49/750.49 (n_e) and 763.26/738.29 (T_e) as non-invasive plasma proxies, validated by high correlation (r > 0.92) with ion probes.

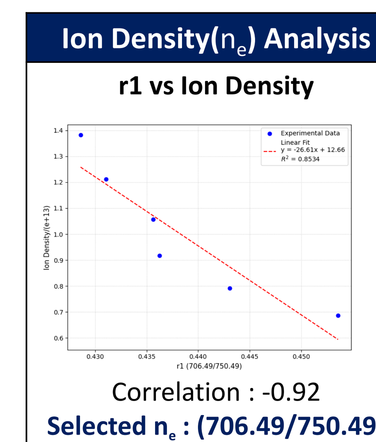
VI variables (9)

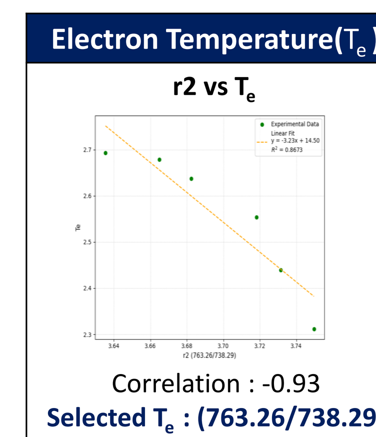
- Transformed raw electrical signals from the multi-frequency bias line into physical kinetics.

Energy Delivery	Power, Reflected power
Ion Acceleration (Energy)	Voltage, Phase
Ion Flux (Density)	Current, Impedance
Surface Reaction	Voltage/Real Ohm Voltage * current Voltage * $\sqrt{Current}$









Feature Selection

PCF (Pearson Correlation Filter)	변수 간 1:1 선형 상관성 산출 → 개별 변수의 직접적 영향력 파악
SVS (Stepwise Vector Selection)	모든 데이터 세트를 학습, 평가 → 최적의 feature 조합 도출
PCA (Principal Component Analysis)	고차원 데이터 행렬의 차원 분해

Forward Strategy

The Bottleneck!
Conventional models faced limits (R2 < 0.82) because dominant OES chemical factors masked crucial physical VI signals.

- Fix dominant chemical factors **(Radical Density)**
- Extract subtle chamber drift from low-variance Principal Components (PC_4~PC_{15}).

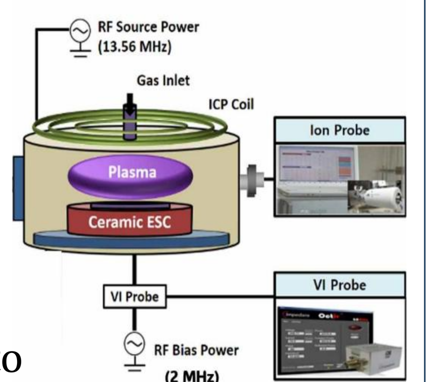
Hybrid VM Model Derivation

3. 식각 메커니즘 고찰 (ETCH MECHANISM)

Chemical Etching

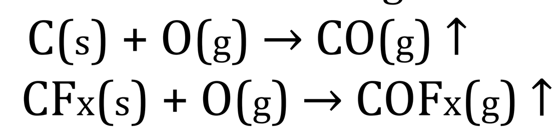
F radicals serve as the primary chemical etchant by reacting with the substrate to form volatile byproducts.

$SiO_2(s) + 4F(g) \rightarrow SiF_4(g)\uparrow + O_2(g)$



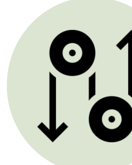
Dual impact of O2 Addition

- liberating effective F radicals and initially increasing the etch rate.
- Excessive O2 flow causes radical over-saturation, leading to active site blocking and heavy non-linear process shifts.



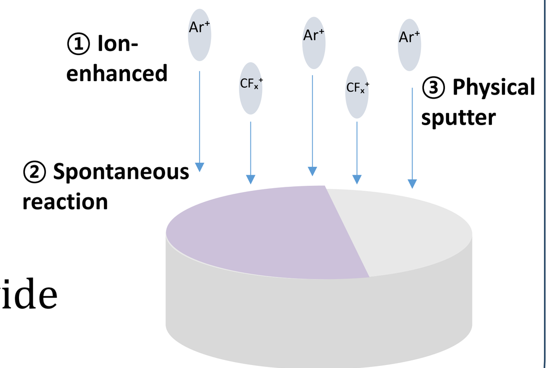
$C(s) + O(g) \rightarrow CO(g)\uparrow$

$CF_x(s) + O(g) \rightarrow COF_x(g)\uparrow$

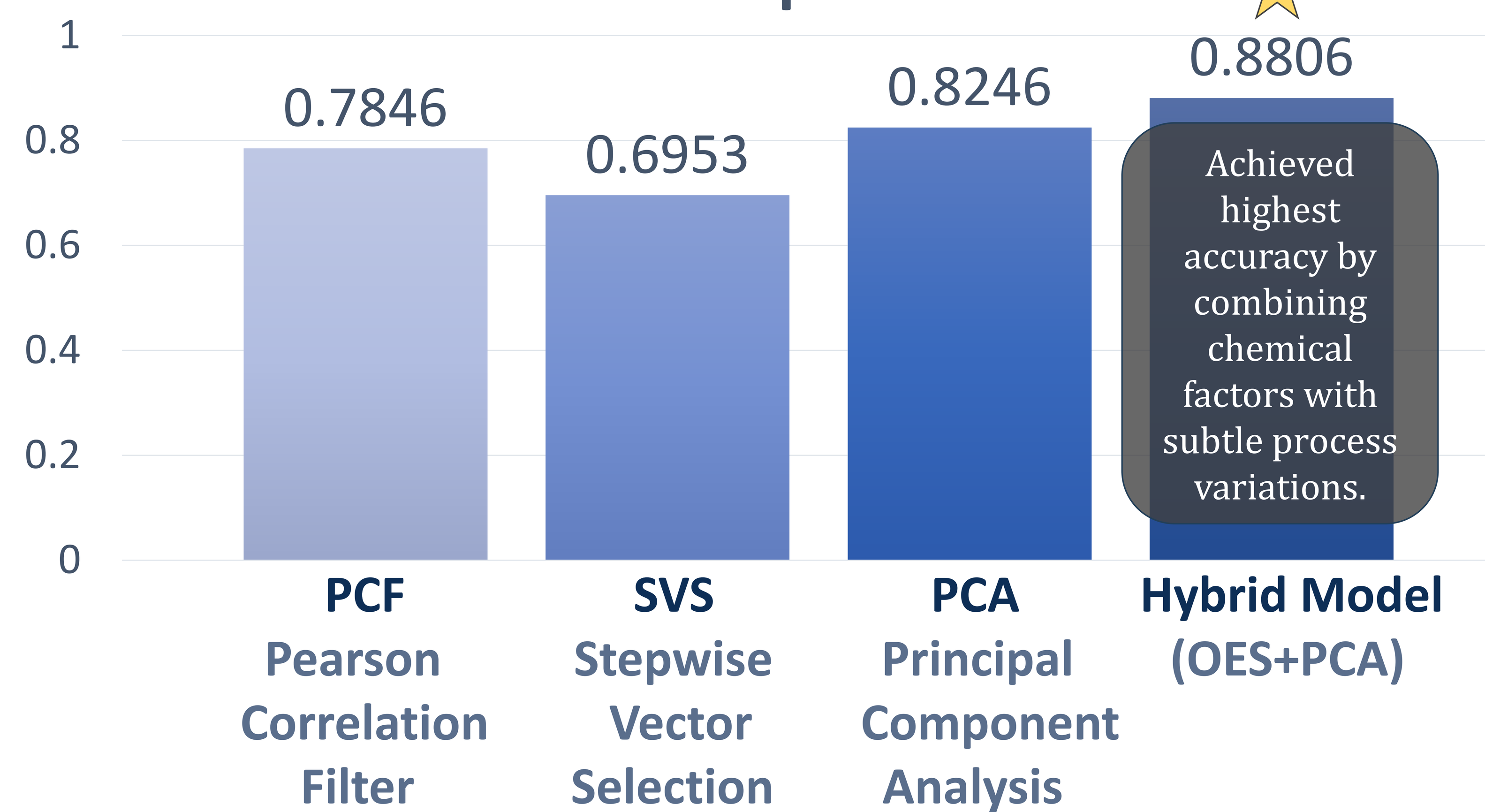


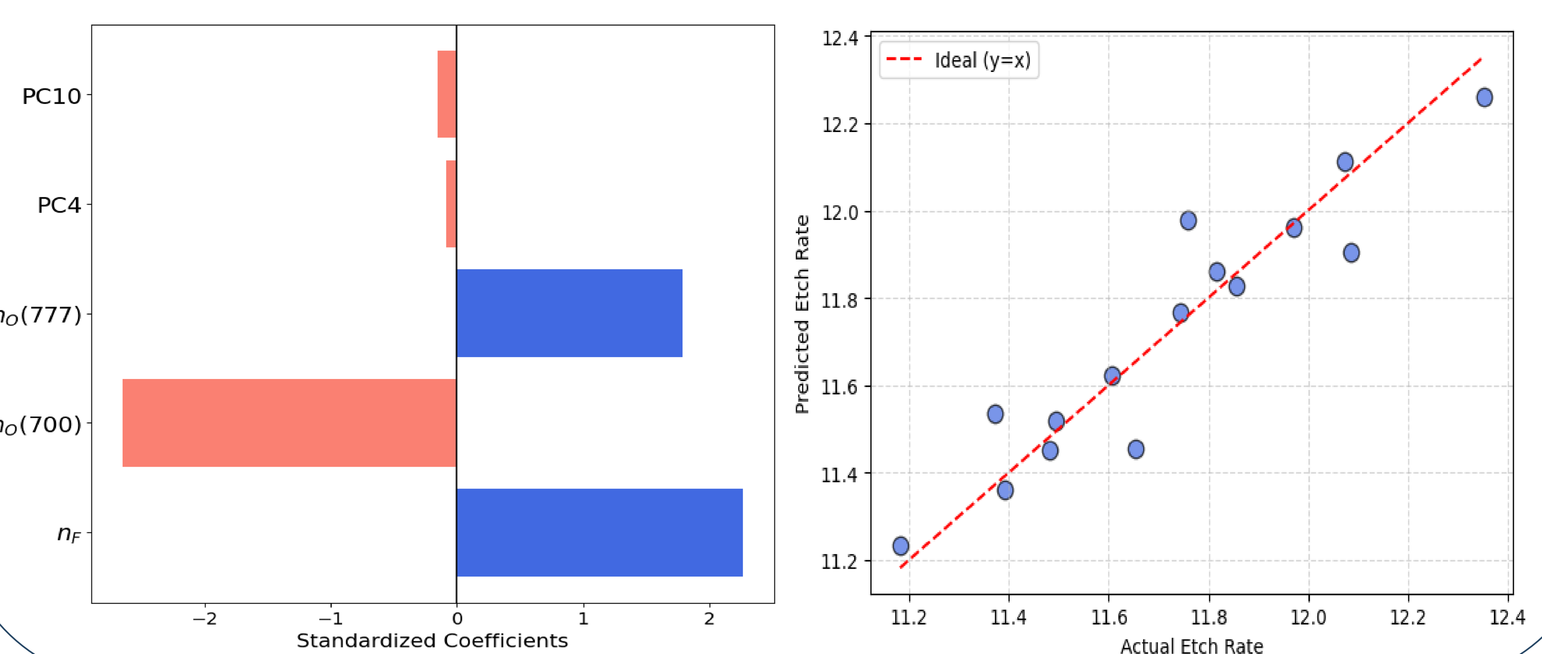
Physical Bombardment

CF_x+ and Ar+ ions driven by bias voltage provide energy bombardment, breaking Si-O bonds and accelerating spontaneous surface reactions.



4. 모델 성능 비교 (RESULTS & DISCUSSION)





결론 (CONCLUSION)

OES (Chemical Quantity) + VI (Physical Quality) → Black Box Explainable

- Demonstrated the importance of physically meaningful variables via OES Actinometry(n_F, n_O).
- Established a hybrid VM pipeline by resolving dependency using independent variables ($PC_{4\sim15}$).
- Improved prediction accuracy to R2=0.88, enabling precise, decorrelated SiO_2 etch rate monitoring.