Advanced materials engineering and stack optimisation of ferroelectric $Al_{1-x}Sc_xN$

Sean McMitchell

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ACTIVE MEMORY

ADVANCED MATERIALS ENGINEERING AND STACK OPTIMISATION OF FERROELECTRIC AL1-XSCXN

Sean McMitchell

17:15 – 17:40 **R109**

OPEN TO:

Globalfoundries, Intel, Sony, TSMC, Samsung, Micron, SKHynix, Qualcomm, Kioxia, WesternDigital, Huawei

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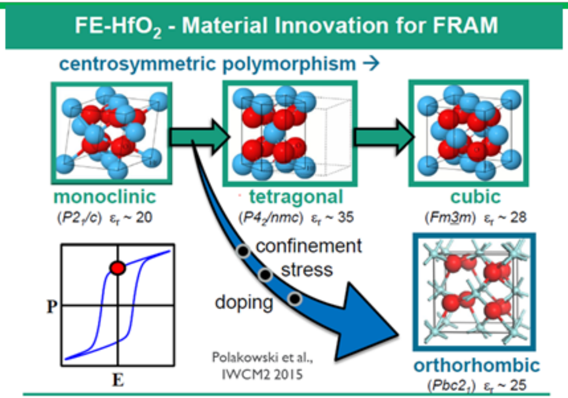
Motivation



Orthorhombic is ferroelectric phase

Advantages

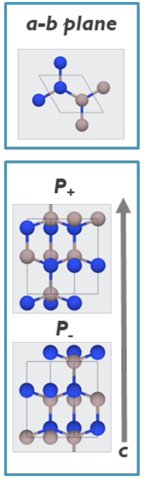
- Scalable to ~5nm
- Fab compatible
- ALD for conformal layers (3D structures)

Disadvantages

- Low P_r (10-20 $\mu C/cm^2$)
- High E_c (2-3MV/cm)
- polymorphic – only up to ~40% ferroelectric
- Phase change with cycling
- Single polarization axis

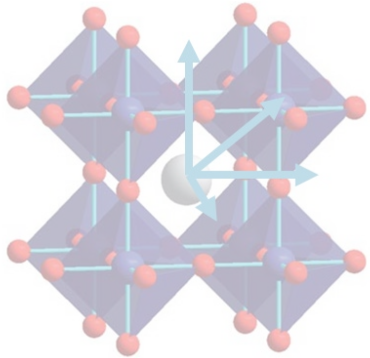
Can we achieve ferroelectricity in other materials at device scale?

Wurtzite Nitrides



- Single phase
- High P_r
- High E_c
- Single polarization axis

Perovskites



- Single phase
- High P_r
- Low E_c
- Multiple polarization axes
- Complex nature
- Low work function

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Executive Summary

- Full CAPA flow demonstrated in $Al_{1-x}Sc_xN$
  - Higher leakage and lower ferroelectric response than Pt-dots
  - Mo and TiN interfaces lower E_c than Pt
- Growth kinetics manipulation explored
  - Releases strain
  - Increases E_c but reduces leakage
- Top electrode stack tuning
  - Mo/Ru/TiN better than Mo only

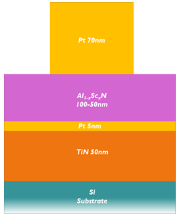
Wurtzites – $Al_{1-x}Sc_xN$ (Pt-dots; coupons)

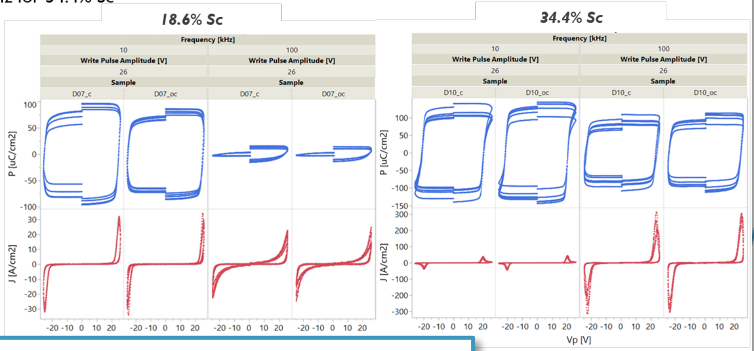
$Al_{1-x}Sc_xN$ - 50nm

E_c too high at 18.6% for full saturation

- PUND used to minimise leakage effects
- Leakage impacts measurement particularly at low Sc% and 10kHz
- Not fully switching at low Sc% → E_c too high
- Full switching at 10kHz for 34.4% Sc

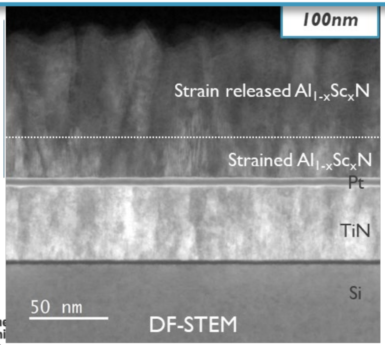
Large Pt-dot capacitors: RC time constant effects seen at higher frequencies





Optimal ferroelectric loops at 34.4% Sc

PTW202104_R112 - McMitchell



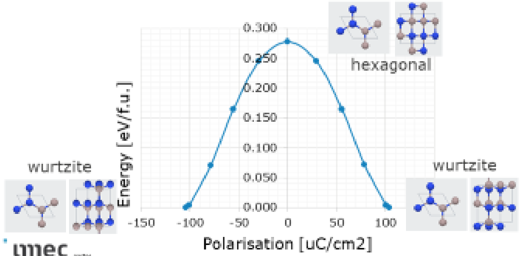
PTW202010_Z101 - Clima

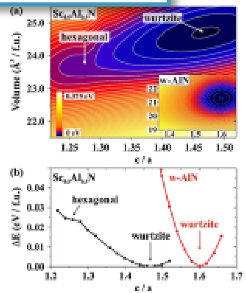
WURTZITE AlN

$P_{AlN} > P_{HfO2}$

High switching barrier W_b=~**270** meV/fu

- Possible to decrease W_b with strain or doping
  - ScAlN[1]
- FE switching crosses a centrosymmetric hexagonal structure





[1] Tasnadi, PRL 104, 137601 (2010)

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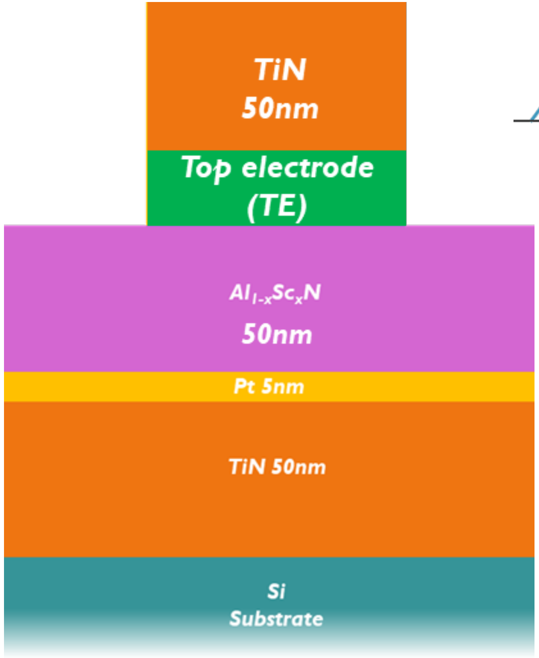
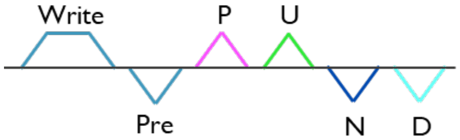
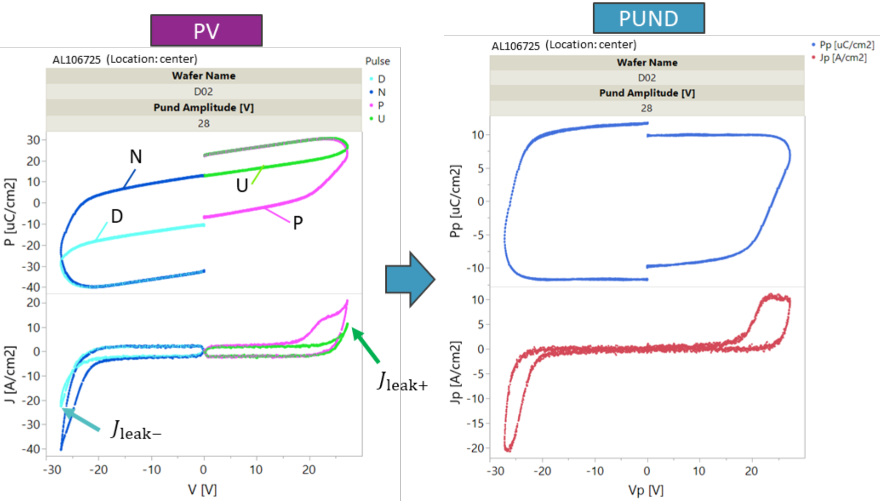
$Al_{1-x}Sc_xN$ - full CAPA flow







- Top electrode: Pt, Ru, Mo
- CAPA flow
- $Al_{1-x}Sc_xN$ grown by PVD co-sputtering

PUND measurements

- PUND waveform
- Write waveform: trapezoid (1μs width)
- Write & read pulse amplitude:
  - 24V, 26V, 28V, & 30V
- Rise + fall time: 5μs + 5μs
  - Single pulse frequency = 100kHz
  - Full wave frequency = 50kHz

- Delay between (write & read) pulses: 1μs
- Device filtering criteria:
- $0\mu C/cm^2 < 2P_r < 400\mu C/cm^2$

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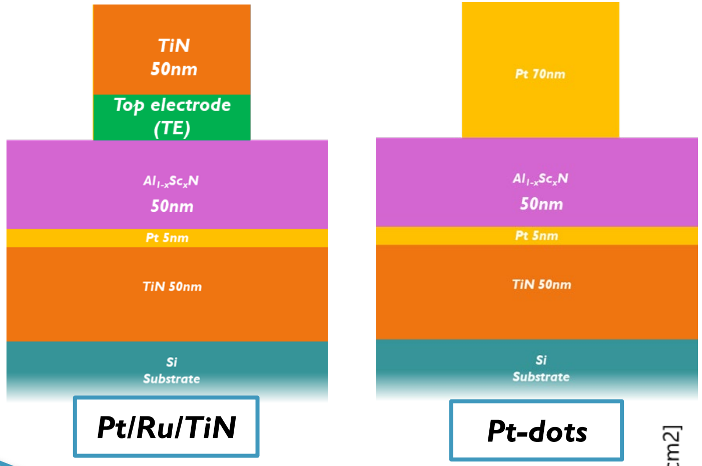
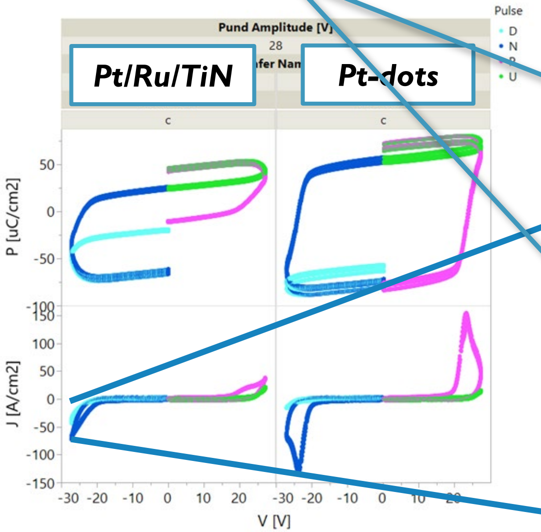
$Al_{1-x}Sc_xN$ - full CAPA flow compared to Pt-dots

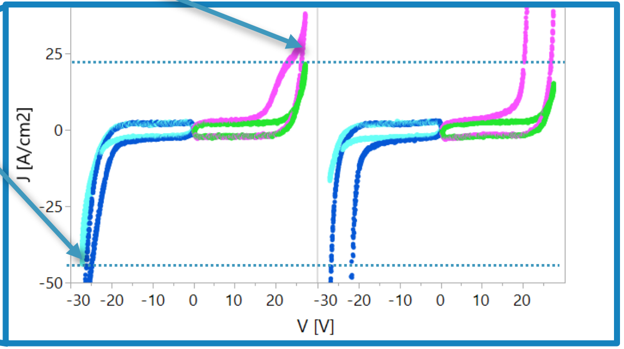
- TE: 5 nm Pt/ 5nm Ru / 50nm TiN
- Reduced $2P_r$ and high leakage → strain and strain gradients

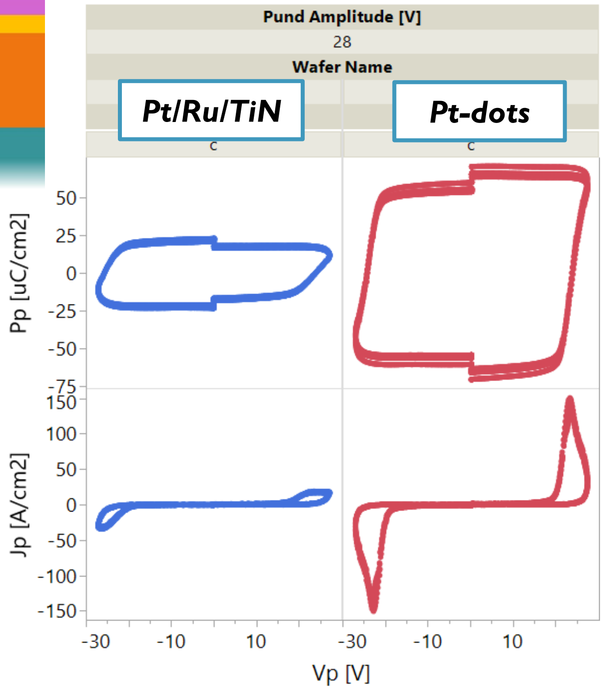
Full flow yields lower $2P_r$ and higher leakage

Slightly larger non-switching current peaks in current lot



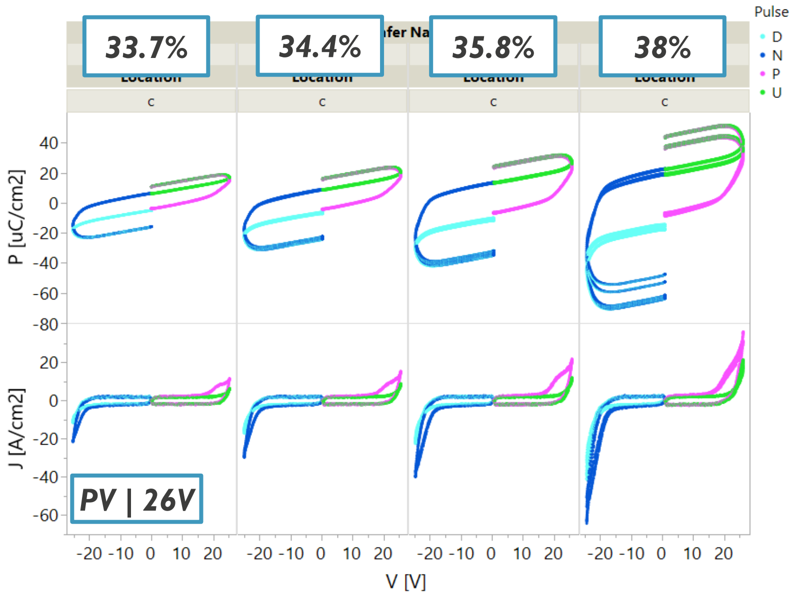


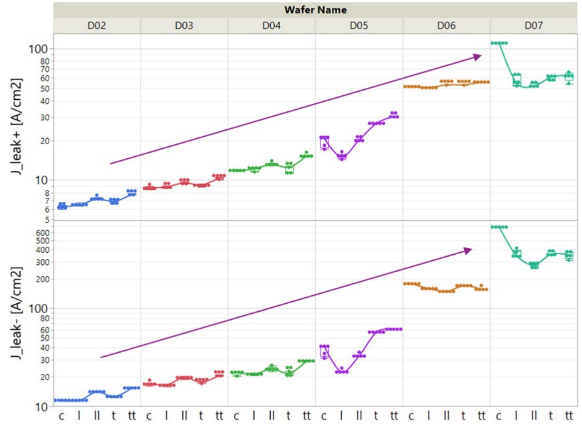


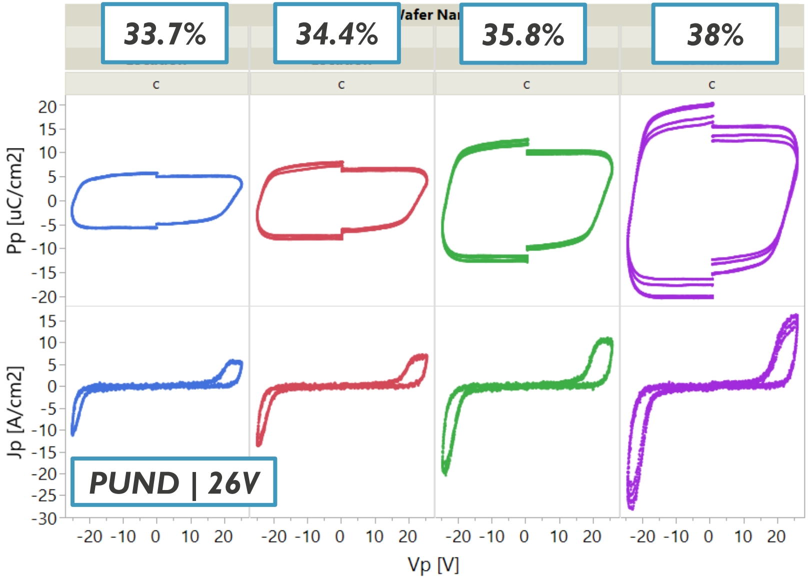


$Al_{1-x}Sc_xN$ - Sc-content

- TE: 5 nm Pt/ 5nm Ru / 50nm TiN
- Leakage increases with Sc%
- Increase in leakage → increase in apparent $2P_r$



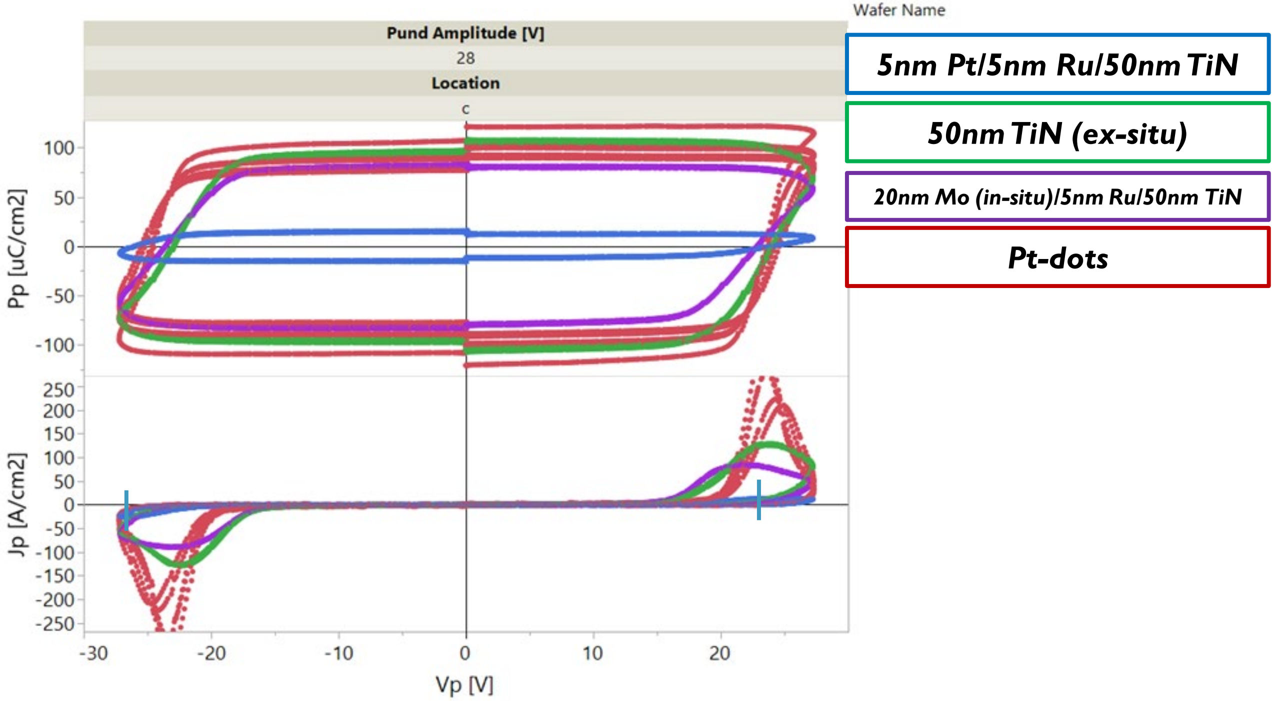




Leakage increases with Sc% → increase in apparent $2P_r$

$Al_{1-x}Sc_xN$ - electrode effects

- Pt-dots show most pronounced switching peak in I-V
- TiN interface lower E_c than Pt-dots but broader ferroelectric response → strain transfer
- Mo interface has lower E_c than TiN interface → strain state



Strain state imposed by top electrode and interface structure at ferroelectric boundary strongly determines ferroelectric properties

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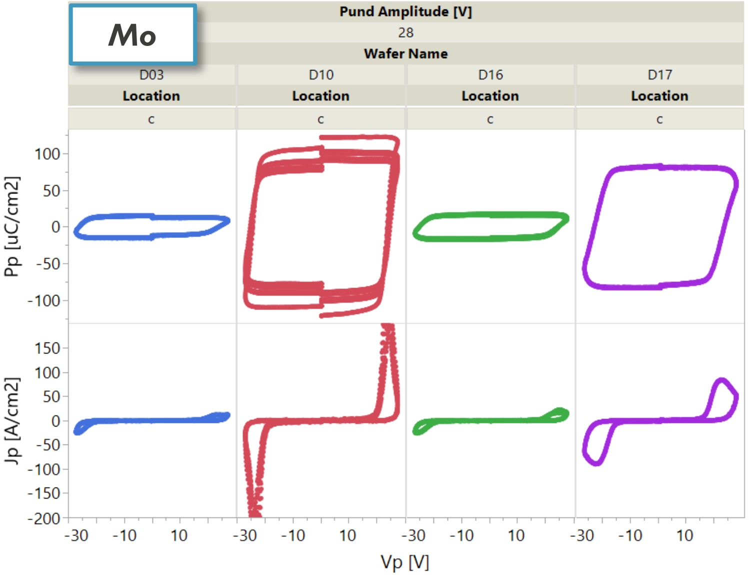
$Al_{1-x}Sc_xN$ - electrode effects

5nm Pt/5nm Ru/50nm TiN

Pt-dots

20nm Mo (ex-situ)/5nm Ru/50nm TiN

20nm Mo (in-situ)/5nm Ru/50nm TiN



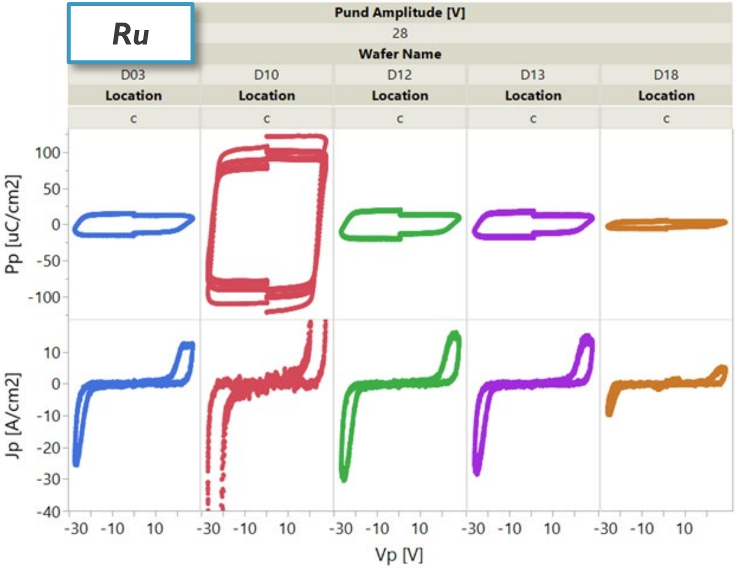
5nm Pt/5nm Ru/50nm TiN

Pt-dots

5nm Ru / 50nm TiN (RIE + IBE)

20nm Ru / 50nm TiN (RIE + IBE)

5nm Ru / 50nm TiN (RIE only)



- In-situ TE deposition important for properties
- In-situ Mo yields best PV → interface structure important (oxidation)
- Apparent drop in $2P_r$ for Ru → reduction of leakage

In-situ deposition of TE to avoid air-break has huge impact on properties

Full flow CAPA towards optimisation

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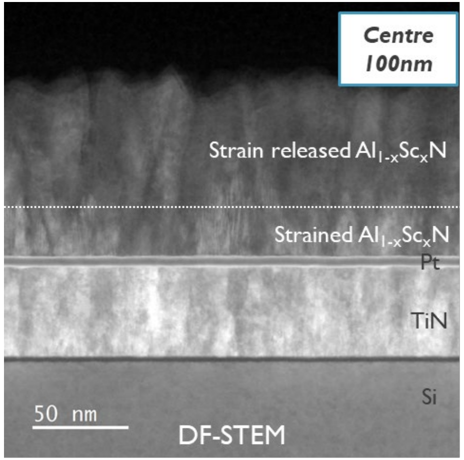
https://doi.org/10.35848/1347-4065/abe644



Full CAPA flow does not match Pt-dot results

- High leakage
  - Switching mechanism generating N-vacancies → step down in bandgap at interfaces
  - Damage from patterning in full flow
- Broadened ferroelectric response and high E_c
  - Strain gradients from microstructure, doping, interfaces → broaden ferroelectric response
  - Strain from varied electrode stack → shifts E_c

Routes to improvement

Growth kinetics engineering

- Use growth rate and kinetics to modify microstructure and strain state

Structural engineering

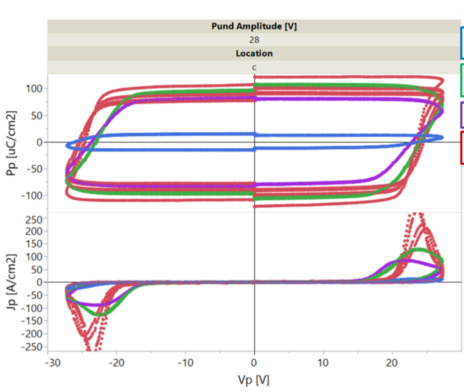
- Interfacial buffer layers of AlN
  - Non-switching so no N-vacancies generated by cycling
  - Same structure as $Al_{1-x}Sc_xN$
  - Can easily feed N into vacancies created at interface during ferroelectric switching reducing bandgap step-down

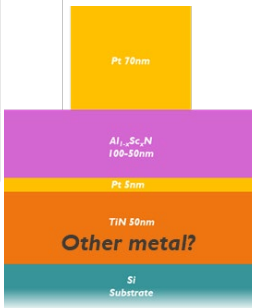
Stack engineering

- Electrode selection
- Replace TiN on BE to change strain without removing Pt-template

Integration

- SSE, Etch conditions, etc. → reduce structural damage



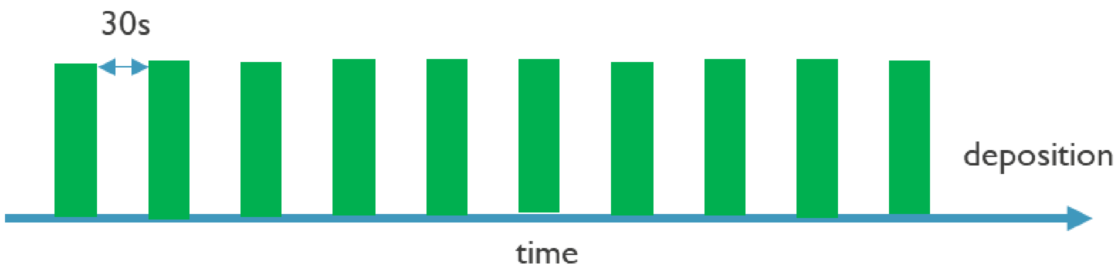


There are still knobs to turn!

Interval deposition and deposition power

Modifying growth kinetics

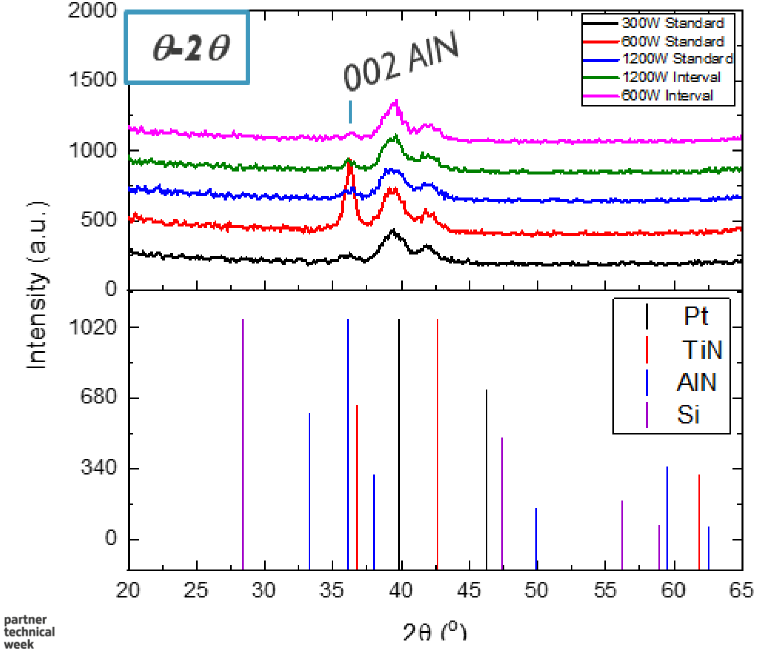
- Interval deposition is used to force 2D growth mode in mismatched systems (typically with pulsed laser deposition) → modifies growth mode and strain state
  - High growth rate to increase supersaturation on growth surface → increases island growth nucleation event probability
  - Intervals of no deposition to allow crystal to arrange
  - Try in PVD for modification of the critical thickness for strain and texture relaxation by growth mode transition (Stranski-Krastinov)
    - 10 intervals of 30s at 1200W (and 600W for comparison)
- Power density on target affects supersaturation, defect formation, microstructure

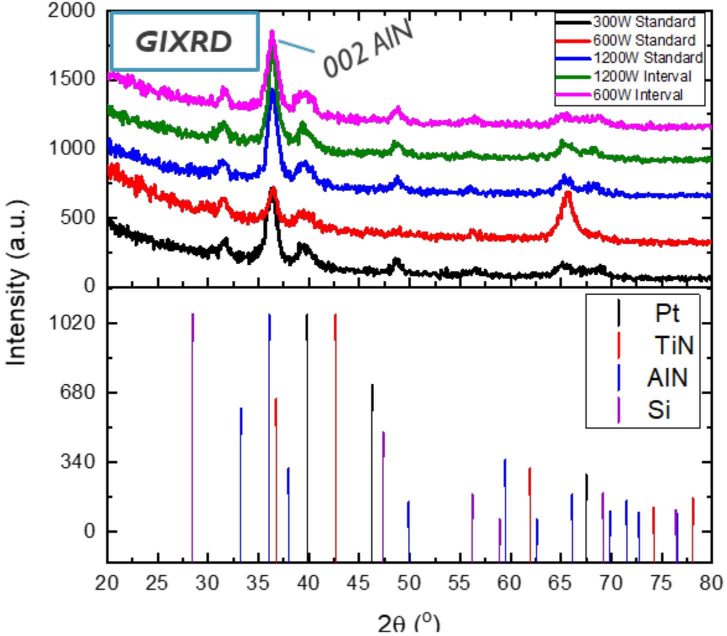


$Al_{1-x}Sc_xN$ - growth kinetics manipulation

- Data shown for 34.4% Sc
- Strongest c-axis texture at 600W standard
- Lower degree of crystallinity from 600W in interval mode
- c-axis texture relaxed when modifying growth kinetics away from standard growth conditions (600W standard)
- c-axis texture relaxation → strain relaxation

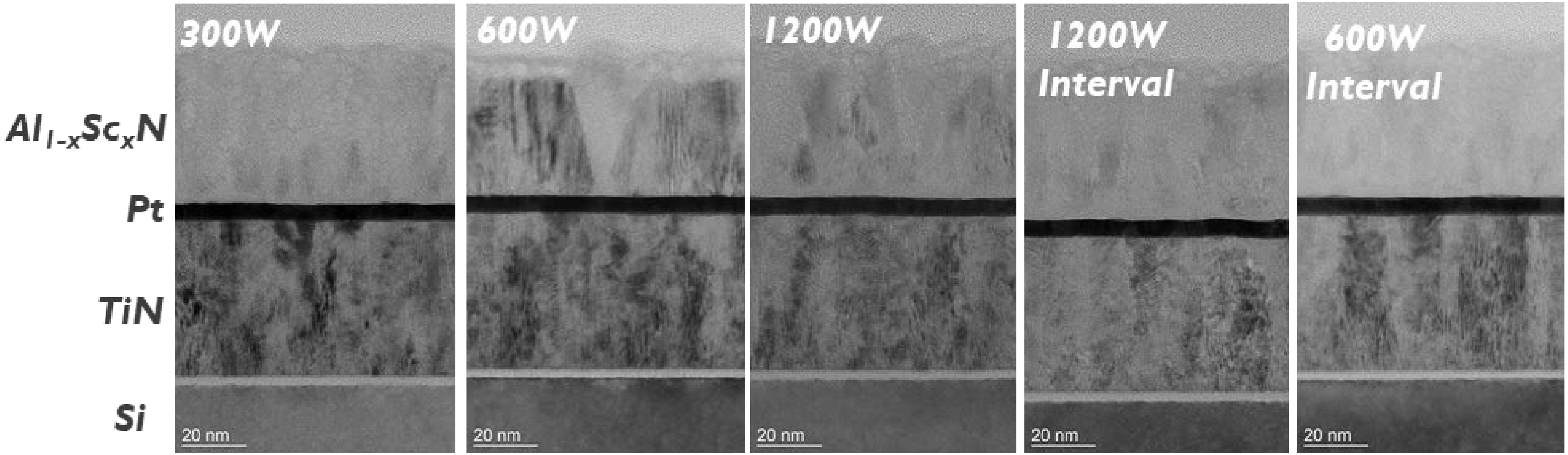
Strain relaxation with modification of growth kinetics





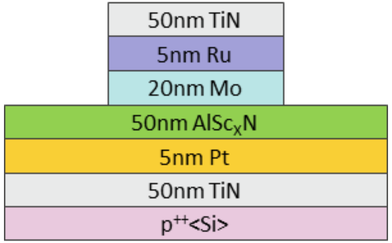
$Al_{1-x}Sc_xN$ - growth kinetics manipulation

- Data shown for 34.4% Sc
- Grain structure more pronounced with 600W and 1200W in standard deposition mode
- High degree of strain fringes seen at 600W in standard mode
- Low power and interval deposition relax grain structure
- Strain fringes are not observed with interval mode

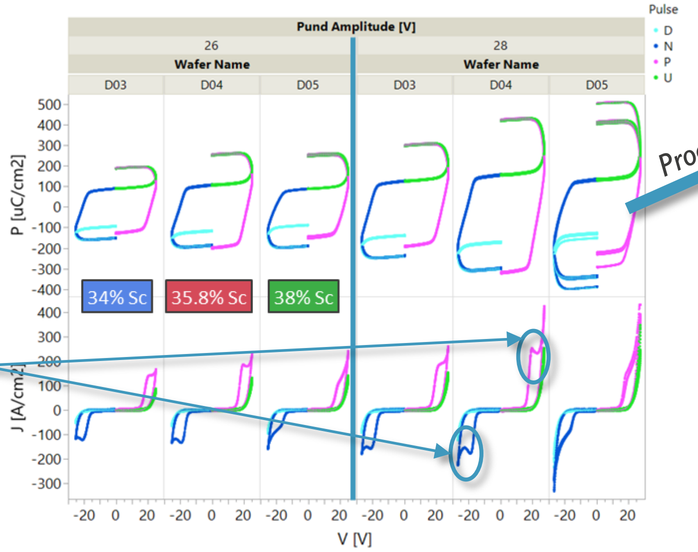


Strain relaxation with modification of growth kinetics

Mo top electrodes



Switching peak most pronounced at 35.8%



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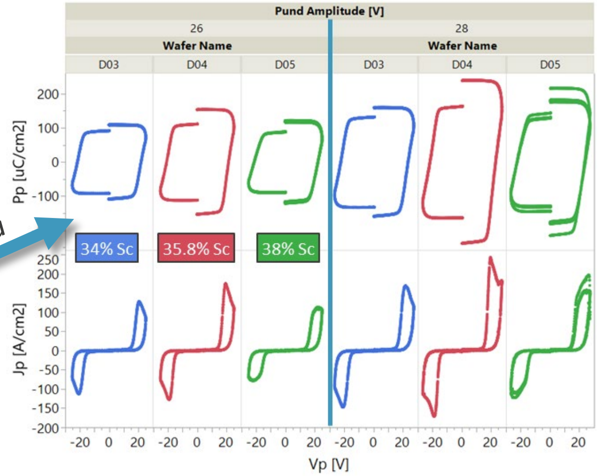
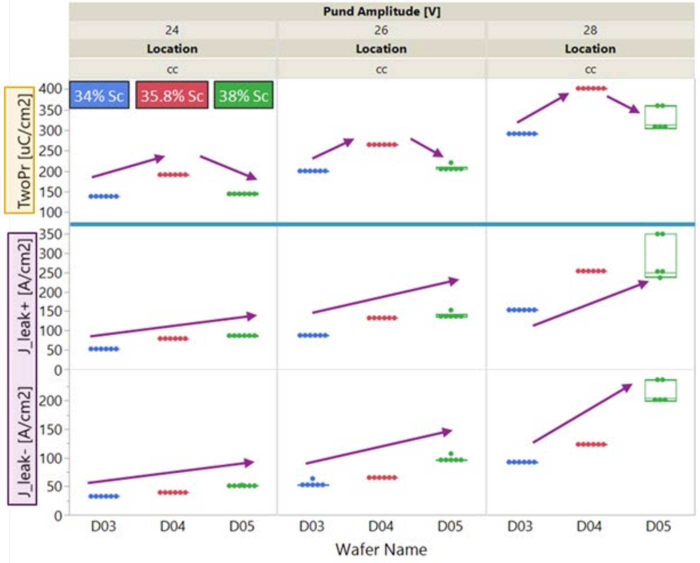


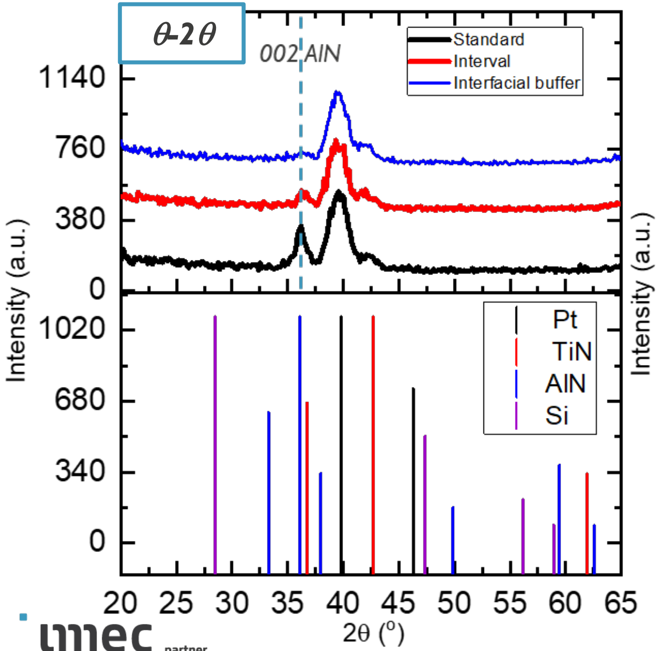


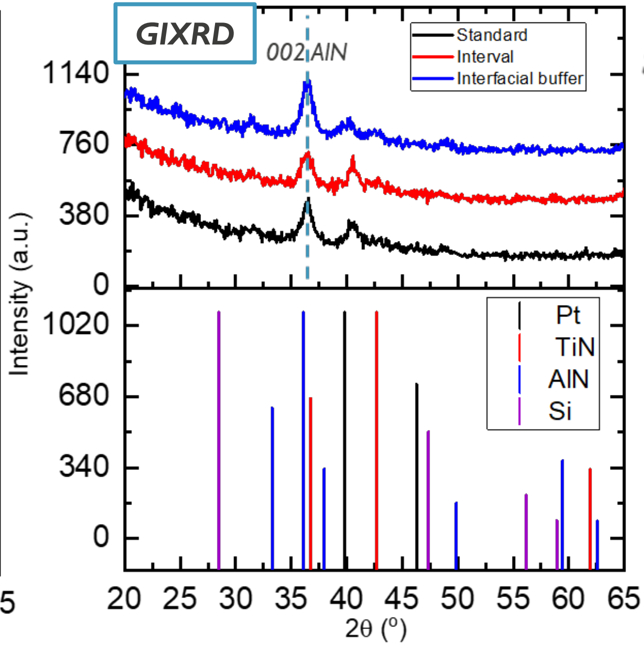
- Standard (600W) deposition
- Increase in leakage with Sc%
- Optimal switching for this thickness and stack at 35.8% Sc (different to with Pt)
- Measured $2P_r$ inflated due leakage contribution

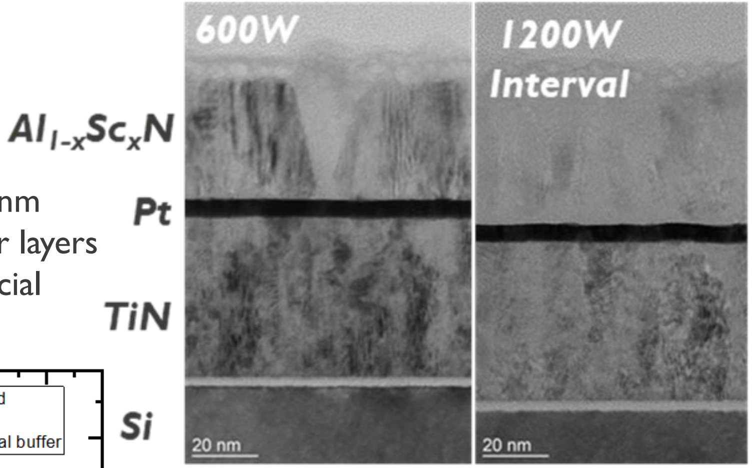
Optimal ferroelectricity at 35.8% Sc

Layer modification

- Data shown for 35.8% Sc
- Interfacial buffer layers: 5 nm AlN → total ferroelectric sandwich thickness 50 nm
- 002 peak shift in θ-2θ indicates relaxation of strain with interval and AlN buffer layers
- c-axis texture strongest with standard deposition → most relaxed with interfacial AlN







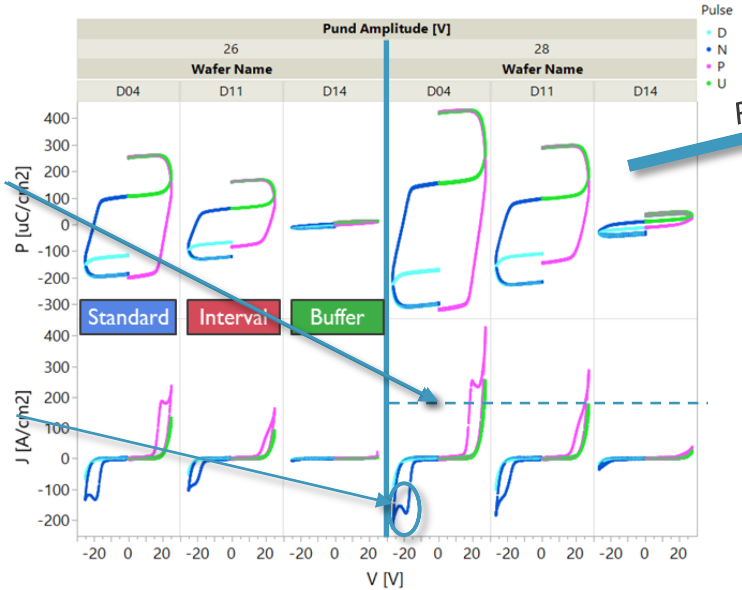
Strain relaxation → texture relaxation

Layer modification

Structural tuning possible → strain from Mo interfaces enhance ferroelectric switching

Leakage (green) highest with standard deposition → lowest with AlN buffer

Switching peak most pronounced with standard deposition



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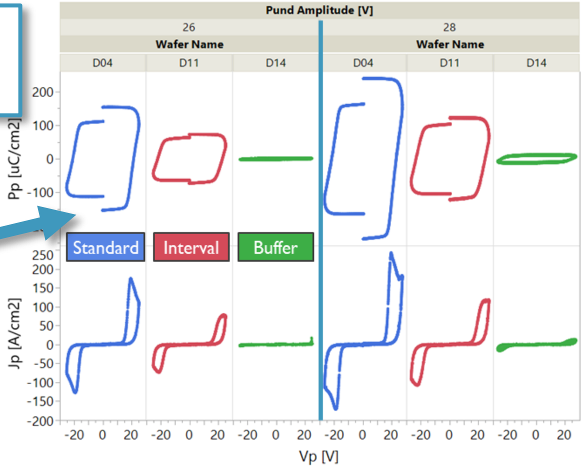
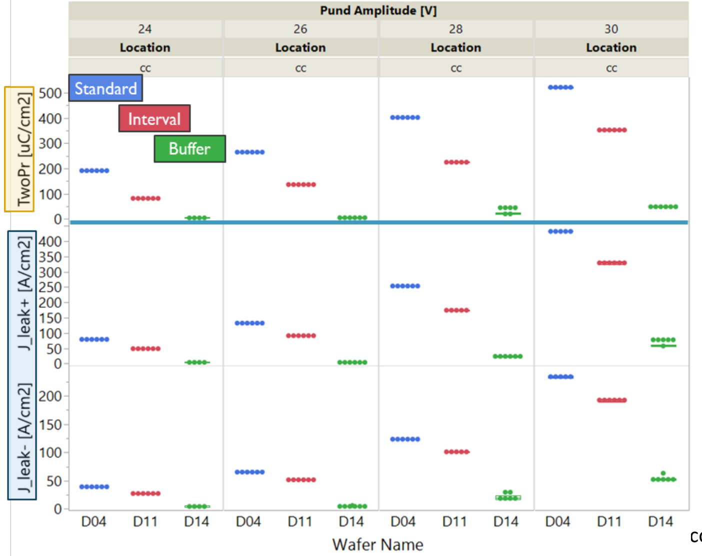
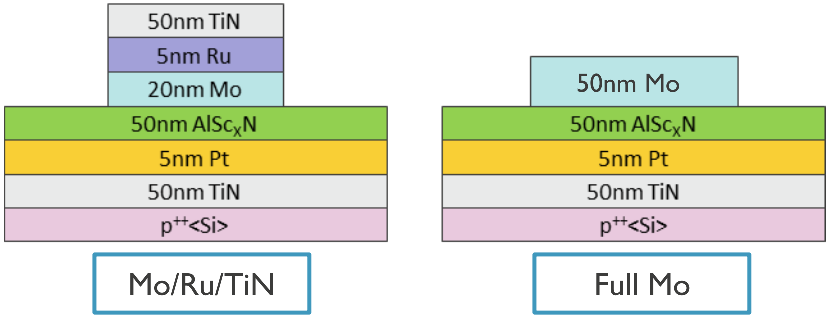


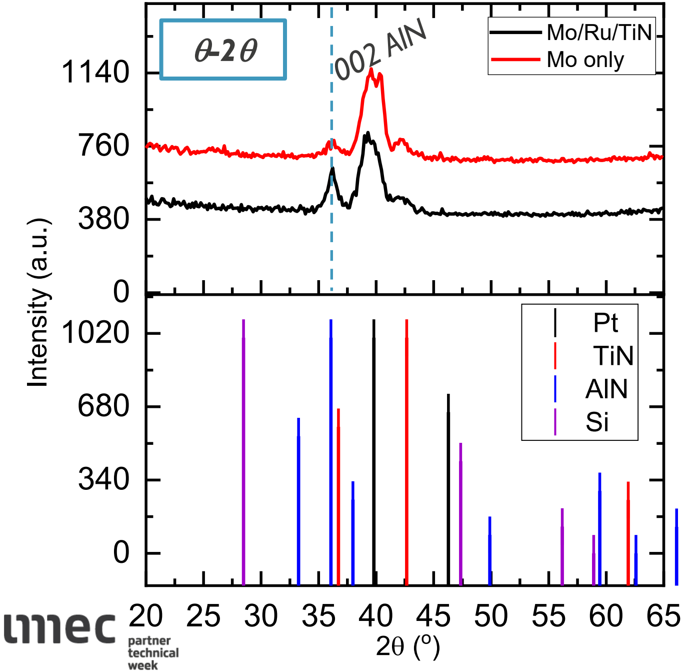


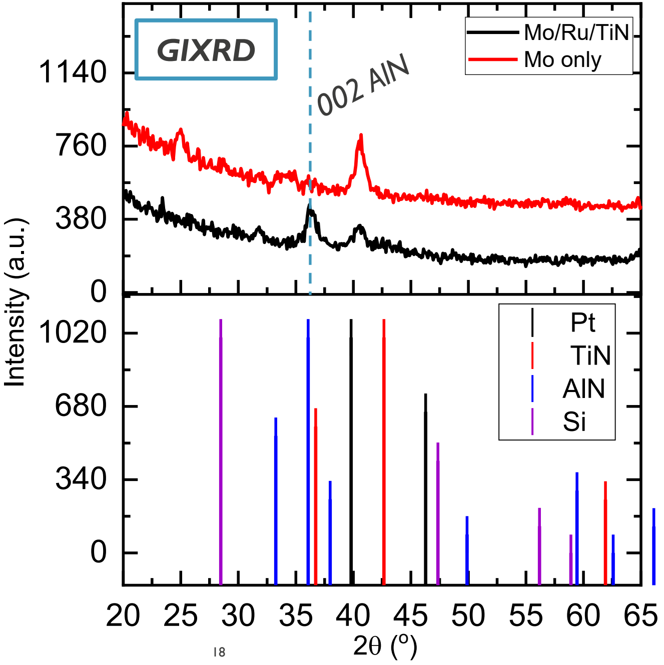
- Standard deposition shows most pronounced ferroelectricity
  - Lower E_c due to higher strain and texture
- Interval deposition yields lower leakage and less ferroelectricity
  - Relaxed texture/strain → better microstructure → fewer leakage paths
  - Higher E_c due to relaxed strain
- AlN buffer layers kill leakage but increases effective E_c

Top electrode stack

- Sharp diffraction peak with the Mo/Ru/TiN electrode → rigid ceramic TiN pinning strain to inhibit strain relaxation → Mo/Ru too thin to fully relax strain
- Broadened 002 peak with full Mo electrodes indicates strain gradients → strain allowed to relax due to malleable electrode material







Strain relaxation dependent on electrode material, thickness, and malleability

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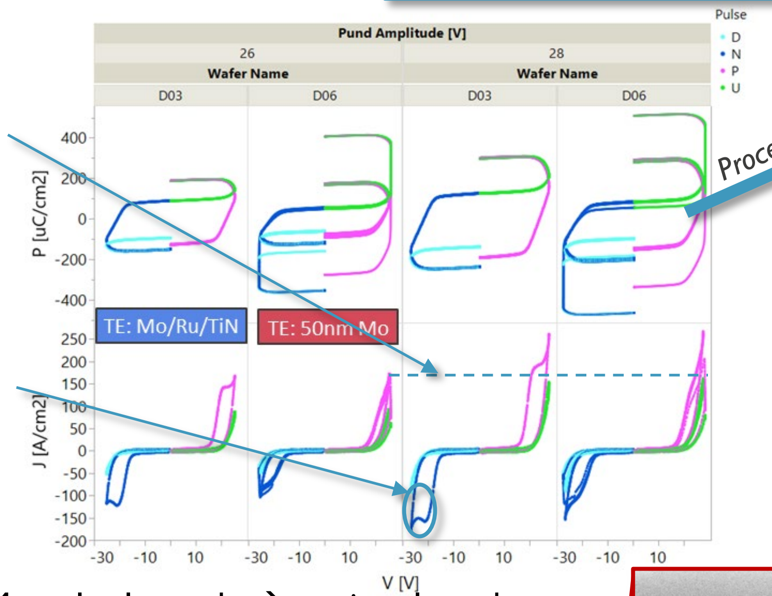
Top electrode stack

Electrode strain can be used to tune E_c

Leakage (green) similar → same interface

Switching peak most pronounced with Mo/Ru/TiN



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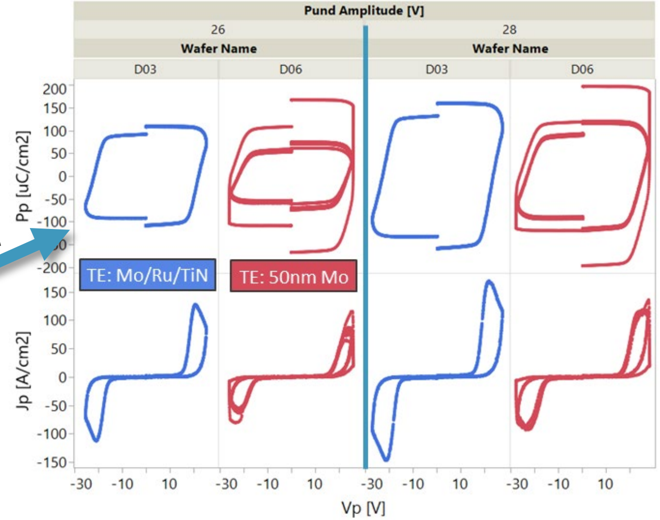
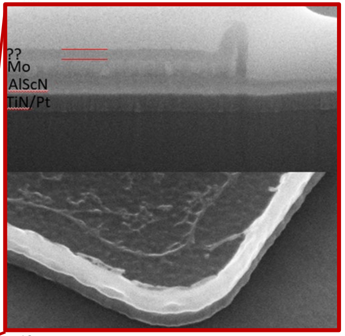
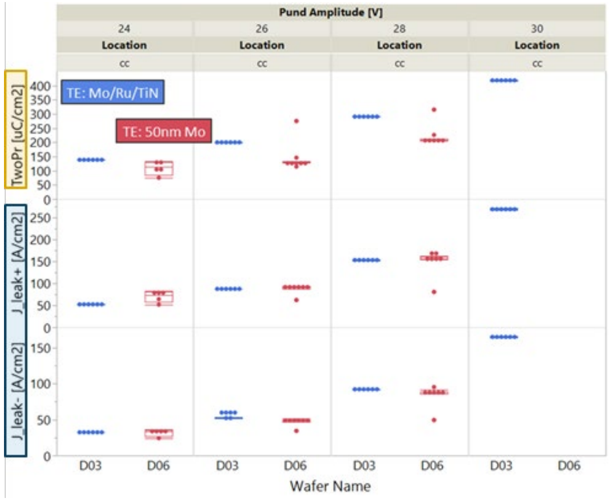


- E_c higher with Mo only electrode → strain released
- E_c lower with Mo/Ru/TiN → rigid TiN pinning strain to shift E_c and enhance switching
- Switching with 50 nm Mo only probably broader in voltage due to strain gradients



Processing issue at etch strip could also cause effective E_c increase with 50nm Mo only



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Conclusions

- Full CAPA flow shows increased leakage and lower ferroelectricity than Pt-dots
  - Strain state
  - Processing
  - Intrinsic leakage from switching mechanism
- Mo and TiN interfaces show best results with lower E_c
- In-situ deposition of top electrodes has big impact on ferroelectricity → no oxidation of wurtzite
- Growth kinetics manipulation releases strain and decreases c-axis texture
- With new BKS (TE: 20nm Mo / 5nm Ru / 50nm TiN) at 50nm thickness 35.8% Sc shows optimal ferroelectricity
- Texture and strain from substrates needed to lower E_c → strain gradients broaden ferroelectric response → releasing strain inhibits switching

Outlook

- Stack optimisation focusing on bottom electrodes
- Growth kinetics tuning closer to standard conditions (600W) for increased strain/texture

Acknowledgements

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Thank you!

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