

Department of
Materials

Electronic and Interface
Materials Laboratory



Characterisation and Understanding of Contact Technology for Terawatt Sustainable Solar Energy

Yuelin Xiong

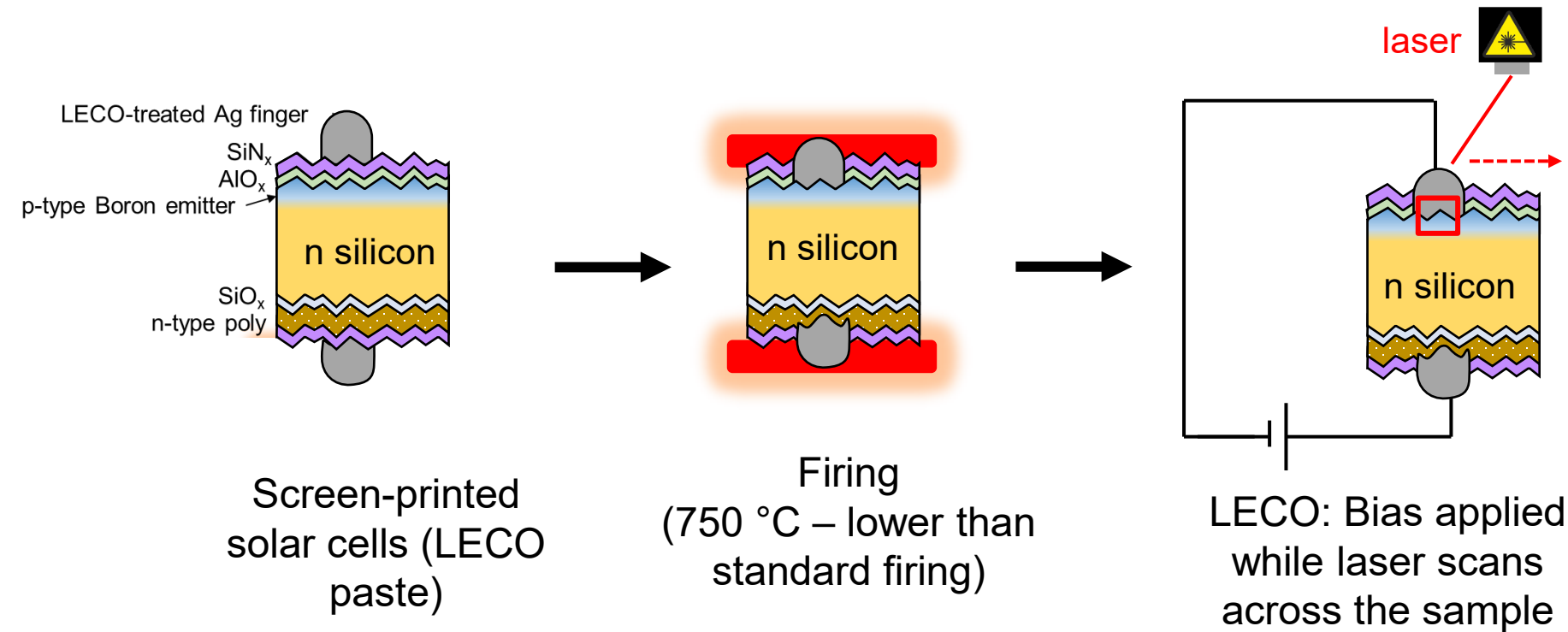
Supervised by: Prof. Ruy Sebastian Bonilla

27th August 2026

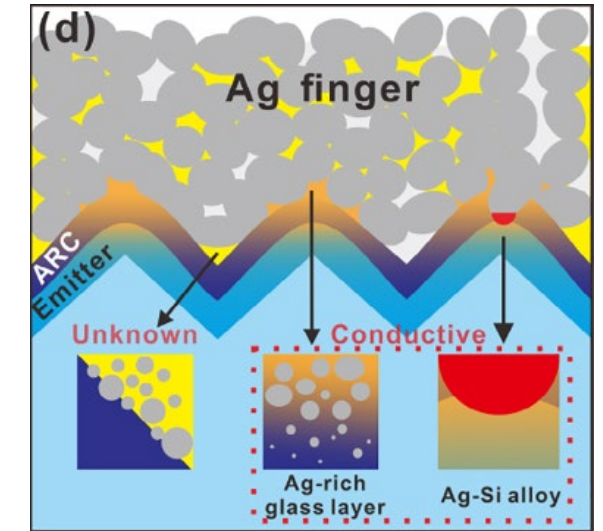


Section 1: Reliability of LECO-treated TOPCon

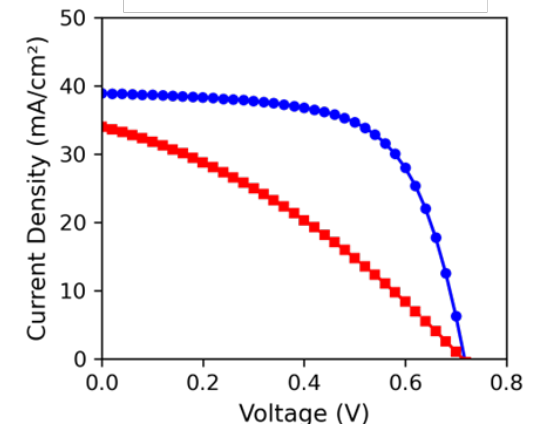
Laser Enhanced Contact Optimisation (LECO)



LECO mechanism:



275 °C 45 mins



η : + 0.26 % abs ρ_c : < 1 mΩ·cm² $J_{0,metal}$: 200 fA/cm²

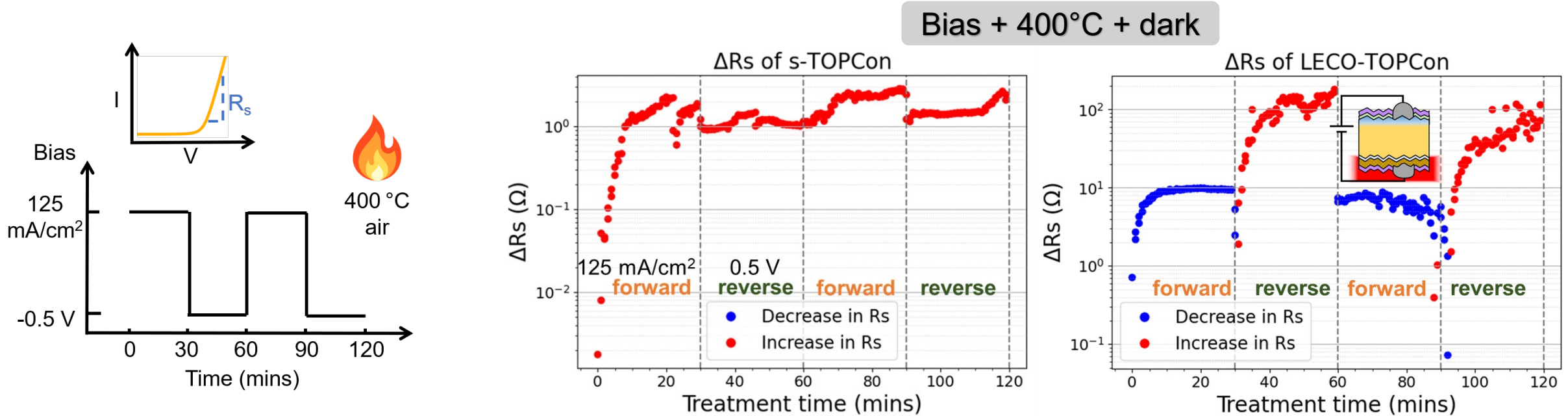
Shi, Z. et al., Solar RRL 10 (2026), e202500932. doi:10.1002/solr.202500932

S. Groser et al., IEEE J. Photovolt., vol. 12, no. 1, pp. 26–30, 2022. doi: 10.1109/JPHOTOV.2021.3129362.

Q. Wang, et al., Progress in Photovoltaics: Research and Applications, 2024, doi: 10.1002/pip.3854.

LECO-treated TOPCon degrades under heat and bias

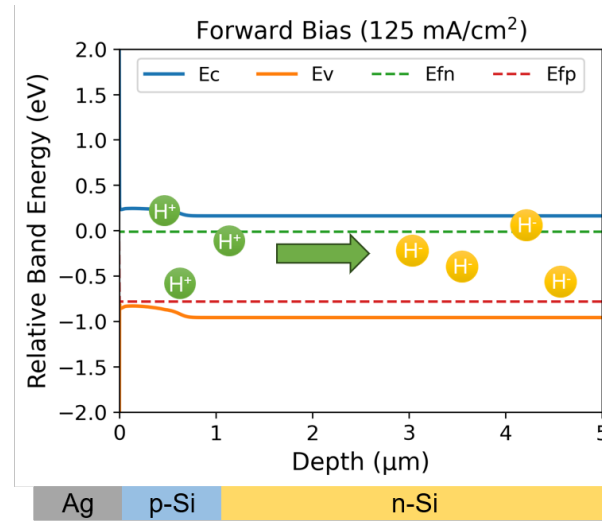
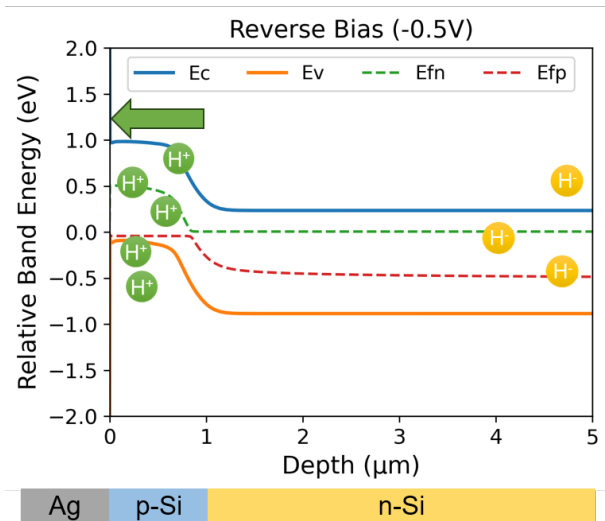
s-TOPCon: standard TOPCon
LECO-TOPCon: LECO treated TOPCon



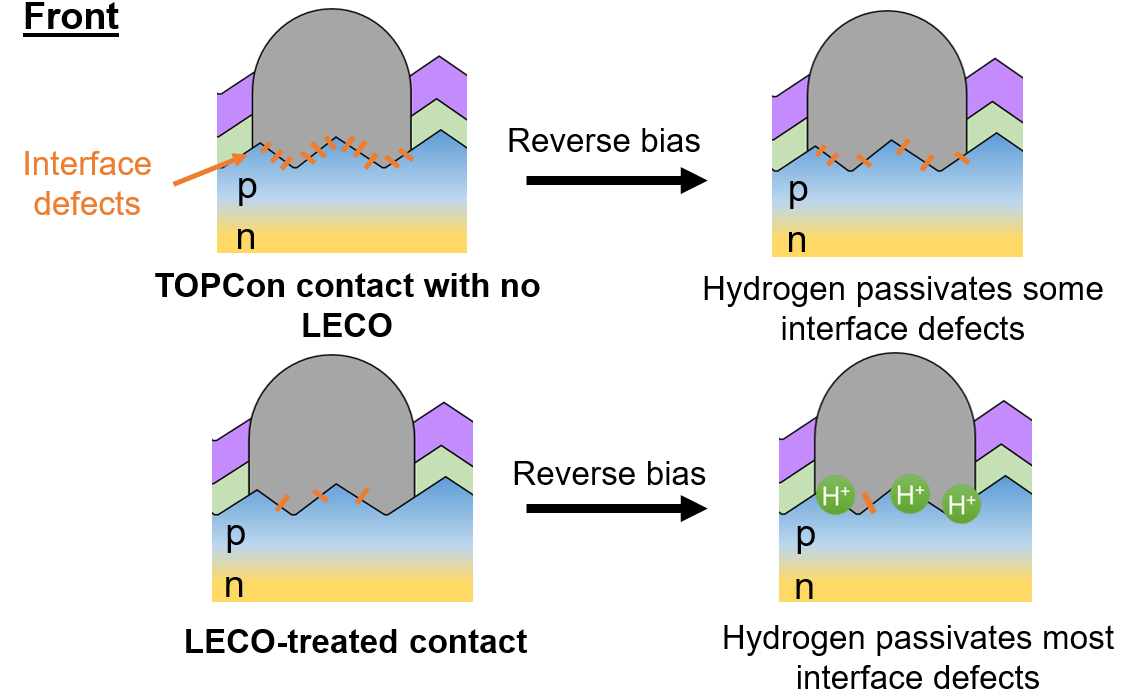
Contact resistivity ρ_c (m Ω ·cm ²)	s-TOPCon (front)	LECO – TOPCon (front)
Before Treatment	9.6	7.6
After Treatment	10.4	511.2

Y. Xiong, *et al.*, *Solar RRL* **9** (2025), 2500151. doi:10.1002/solr.202500151

Hypothesis: hydrogen-related degradation



Front

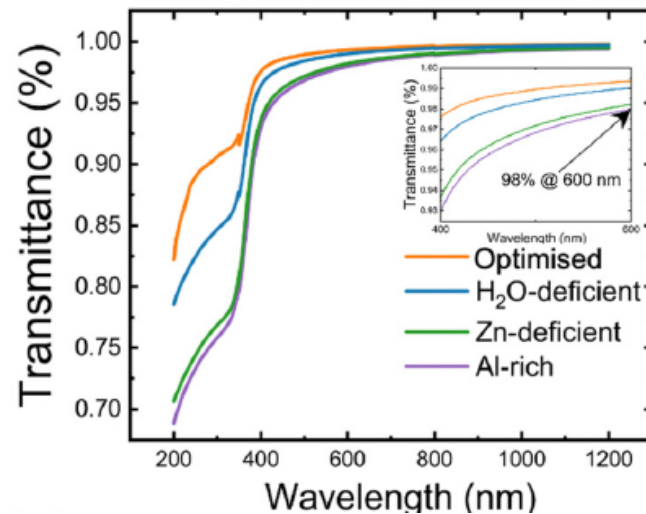


Section 2: Linking doped-ZnO properties to microstructure

Aluminium-doped zinc oxide (AZO) – A trinity of useful properties

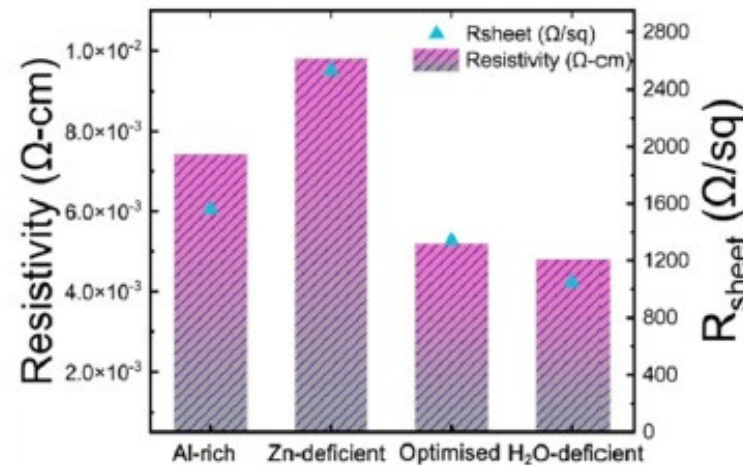
Indium-free TCO

Transparent?
(40 nm AZO)



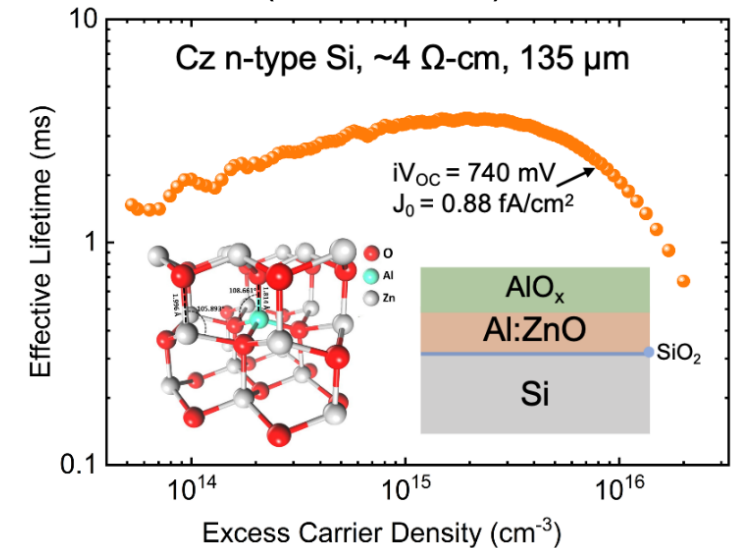
ITO Transmittance = 82-87% at 600 nm wavelength (50 nm ITO)

Conductive?
(50 nm AZO)



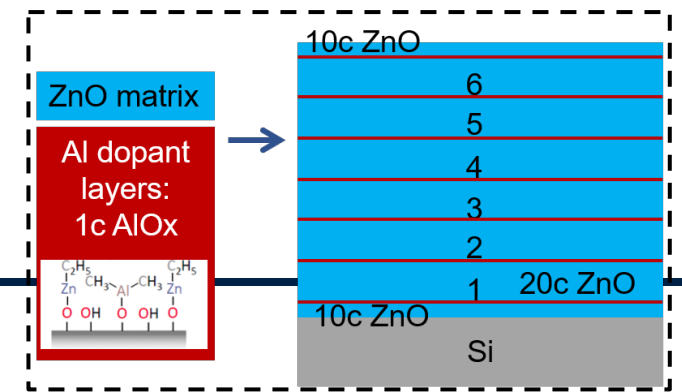
ITO resistivity = 0.6×10^{-3} ohm cm

Passivating?
(20 nm AZO)



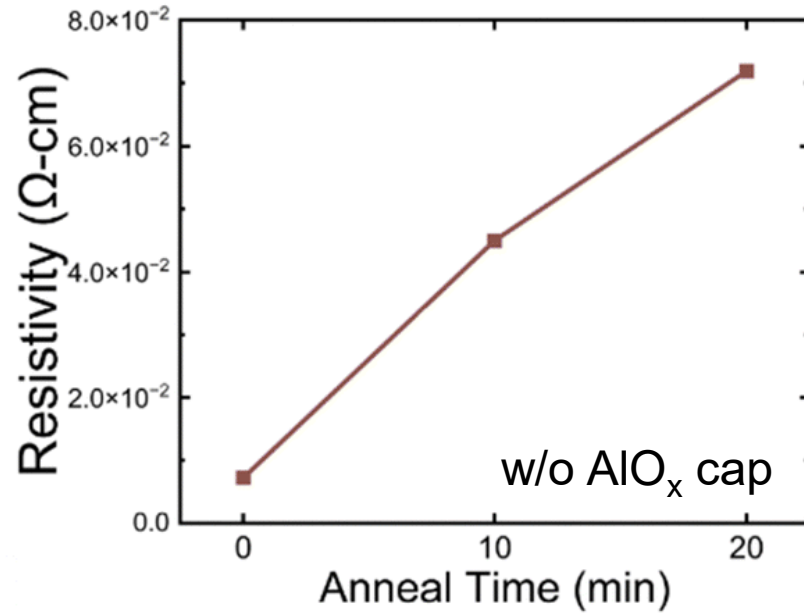
AZO offers a low-cost, indium-free TCO with competitive optical and electrical properties — enabling scalable tandem solar cells.

Yan Wang, *Energy Adv., Advance Article* (2025).

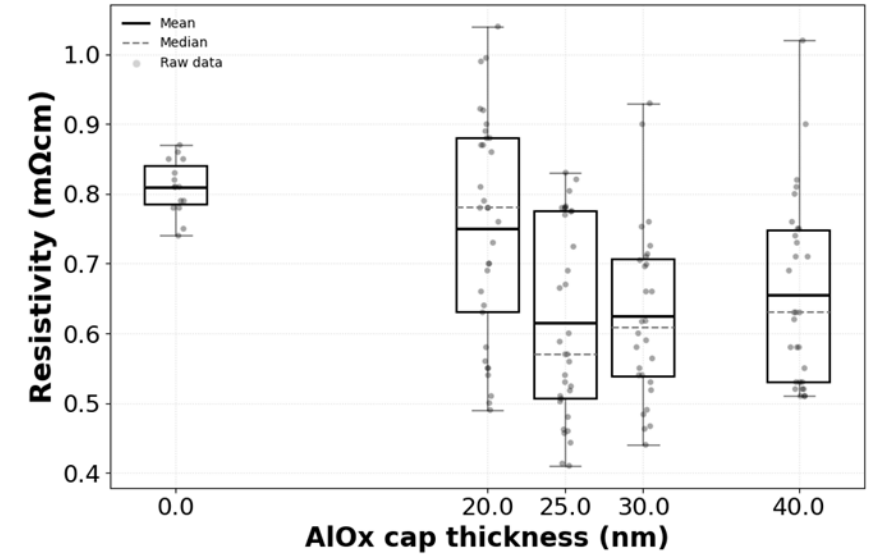
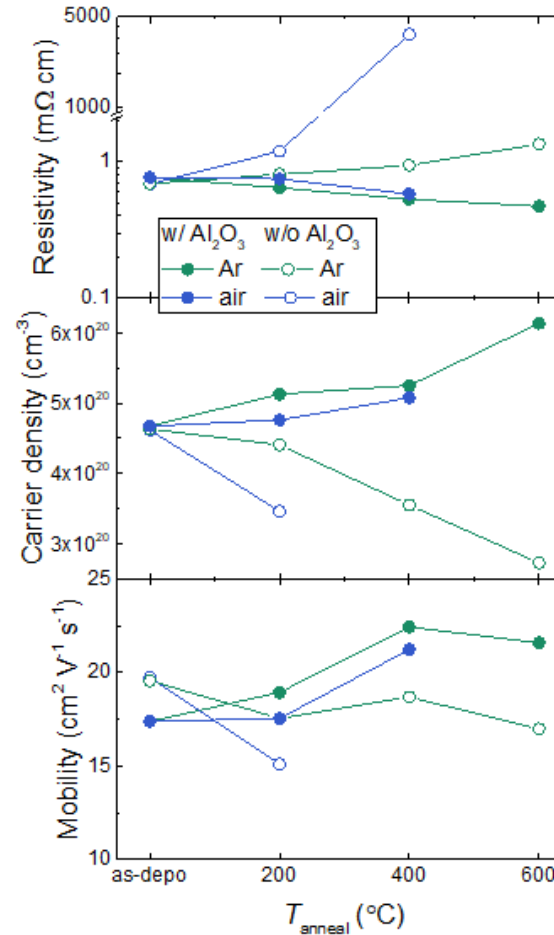


Annealing changes the electrical properties of doped ZnO

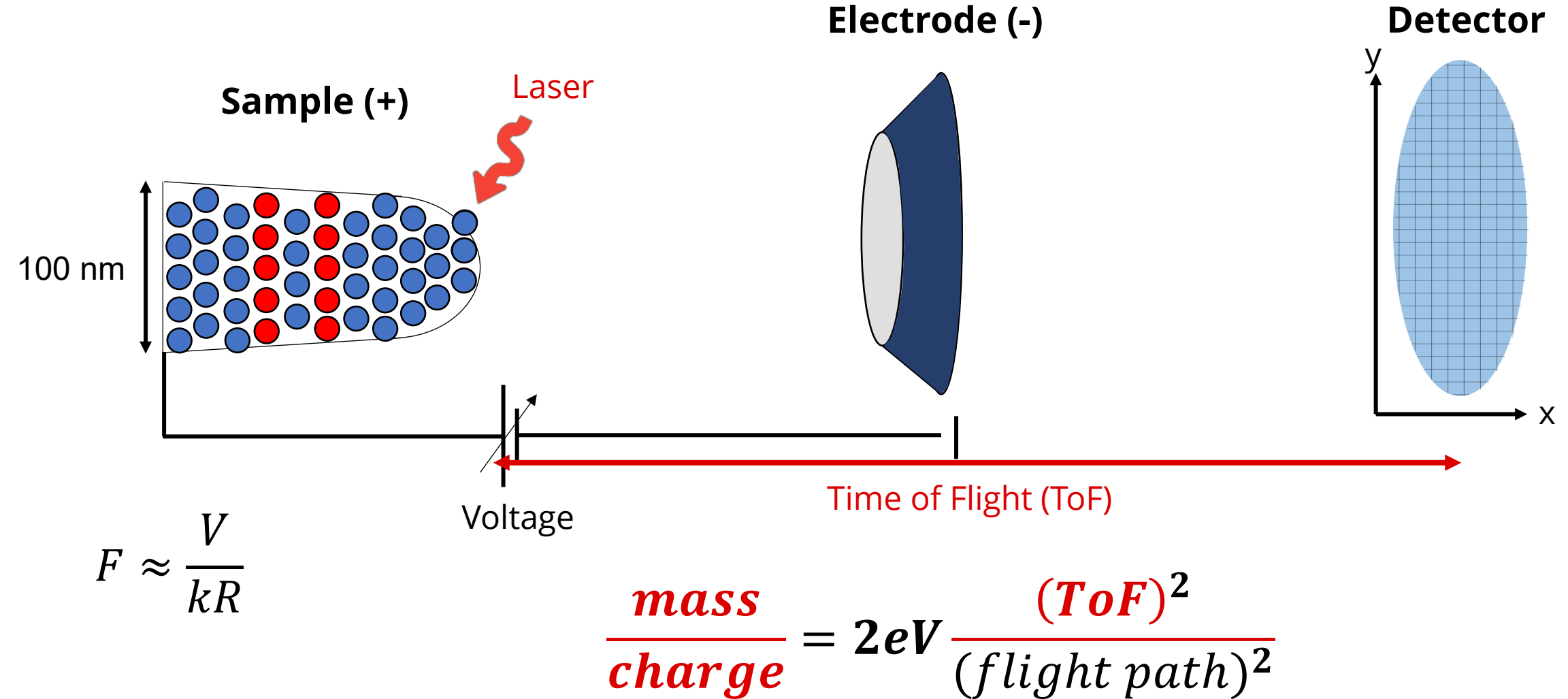
Al-doped ZnO



Ga-doped ZnO



Atom Probe Tomography (APT)

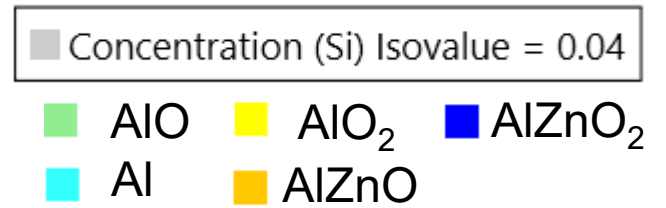


Why use APT?

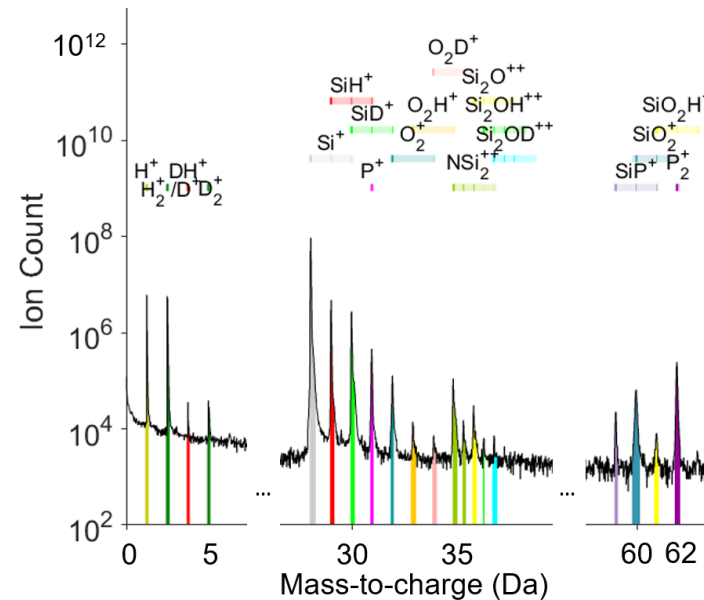
1. Position information in x,y,z
2. Mass to charge state ratio from ToF

Strengths of APT

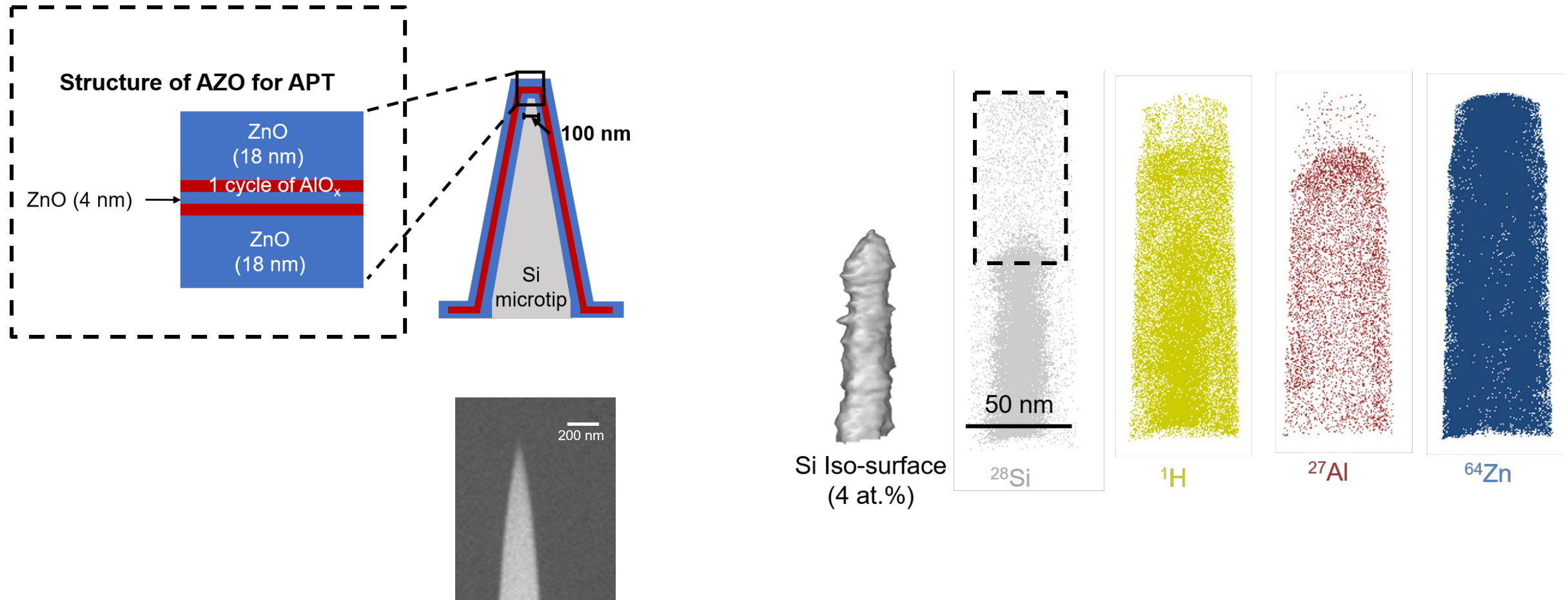
- Very high, almost atomic scale resolution
- Visualising 3D nanostructure
- Equally sensitive to all elements



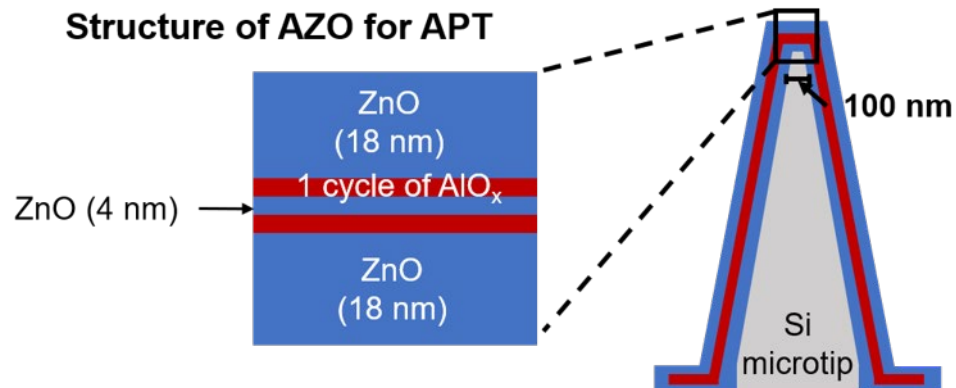
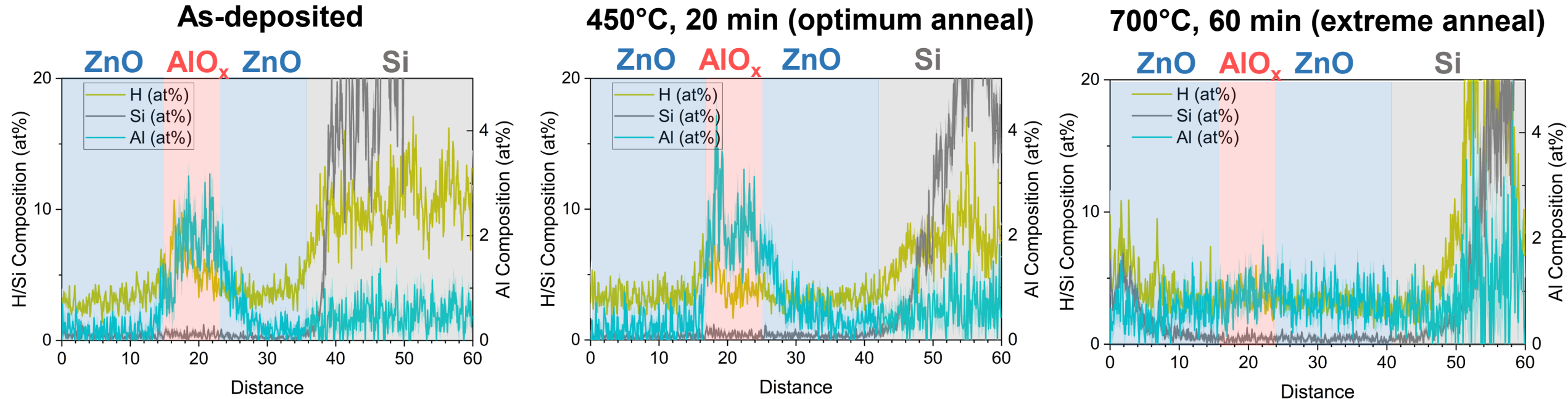
3D
reconstruction:



Sample structure and elemental distribution of AZO



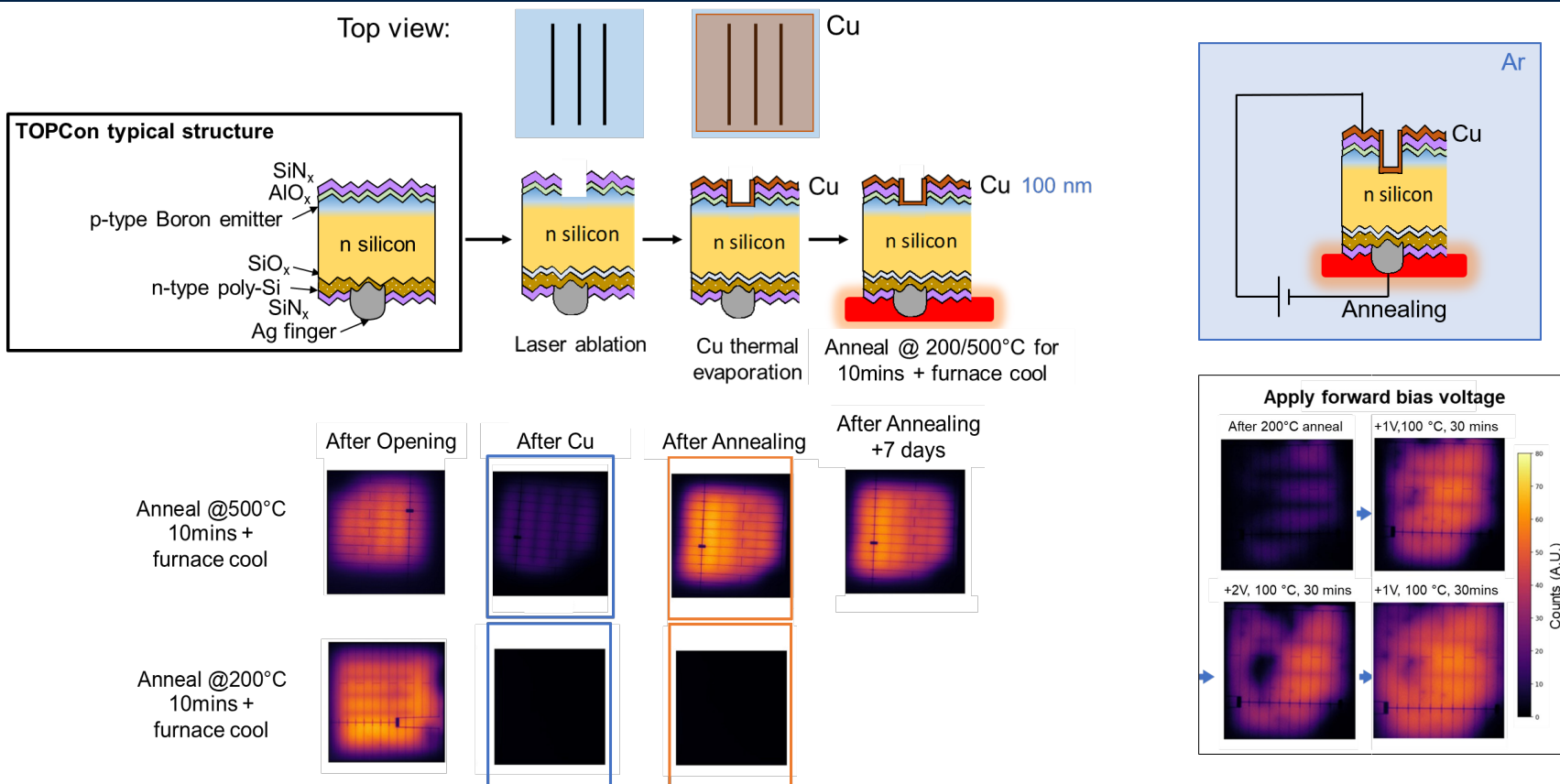
Effect of annealing on dopant distribution in AZO



- **450°C, 20 min:** minimal Al redistribution; H remains concentrated near the AlO_x layer.
- **700°C, 60 min:** H and Al redistribute strongly.
- Dopant redistribution $\neq$ carrier transport.

Section 3: Copper metallisation and defect characterisation

Characterisation of Cu/Si interface in TOPCon



Slow cooling
→ Fewer, larger Cu precipitates [1,3].
→ Some Cu may remain interstitial [1,2].

Cu out-diffusion
→ Cu migrates to surfaces or B-doped Si [4].

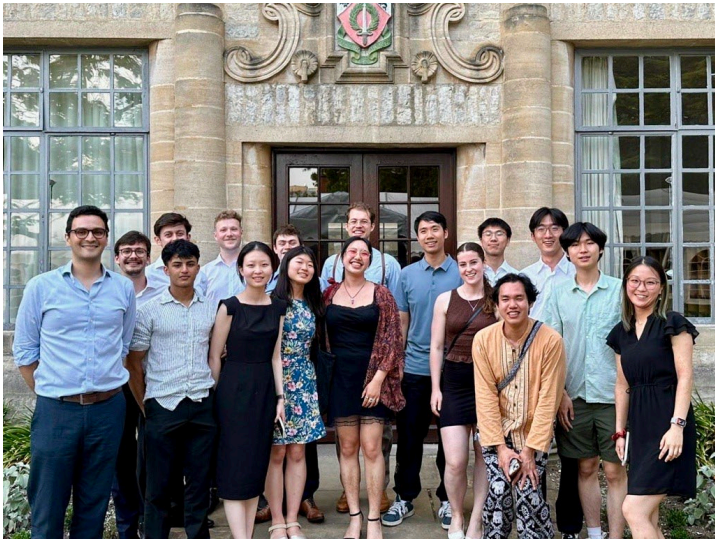
- [1] Istratov & Weber, *JES* (2002).
- [2] Istratov & Weber, *Appl. Phys. A* (1998).
- [3] Seibt et al., *phys. stat. sol. (a)* (1999).
- [4] Shabani et al., *JES* (1996).

Characterisation of Cu defects:

- Low-temperature PL: Only detects radiative defects; the 1.014 eV Copper line depends on the type of Cu complex.
- DLTS: Requires a junction/depletion region; difficult on finished devices.
- Time and Injection-dependent Lifetime Spectroscopy (TIDLS): Requires lifetime measurements; difficult after metallisation.

Acknowledgements

Many thanks to



Electronic and Interface
Materials Laboratory



Oxford Atom Probe Group

Thank you to everyone at SPREE for welcoming me to UNSW.

Special thanks to Umair, Shona, Ziv, Shuai and Ali, and to the ACDC Group.

Funded by

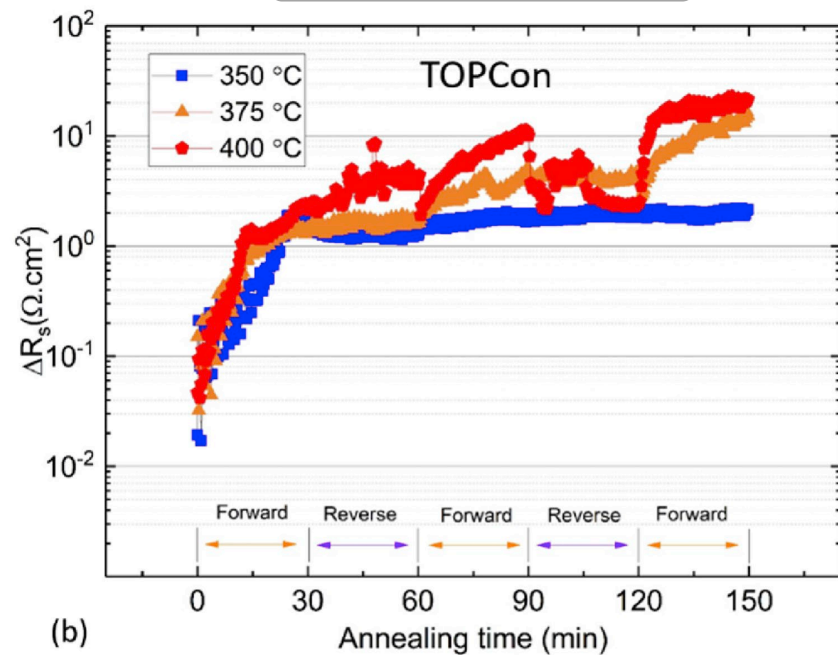


Email: yuelin.xiong@materials.ox.ac.uk
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Thank you!

Supplementary

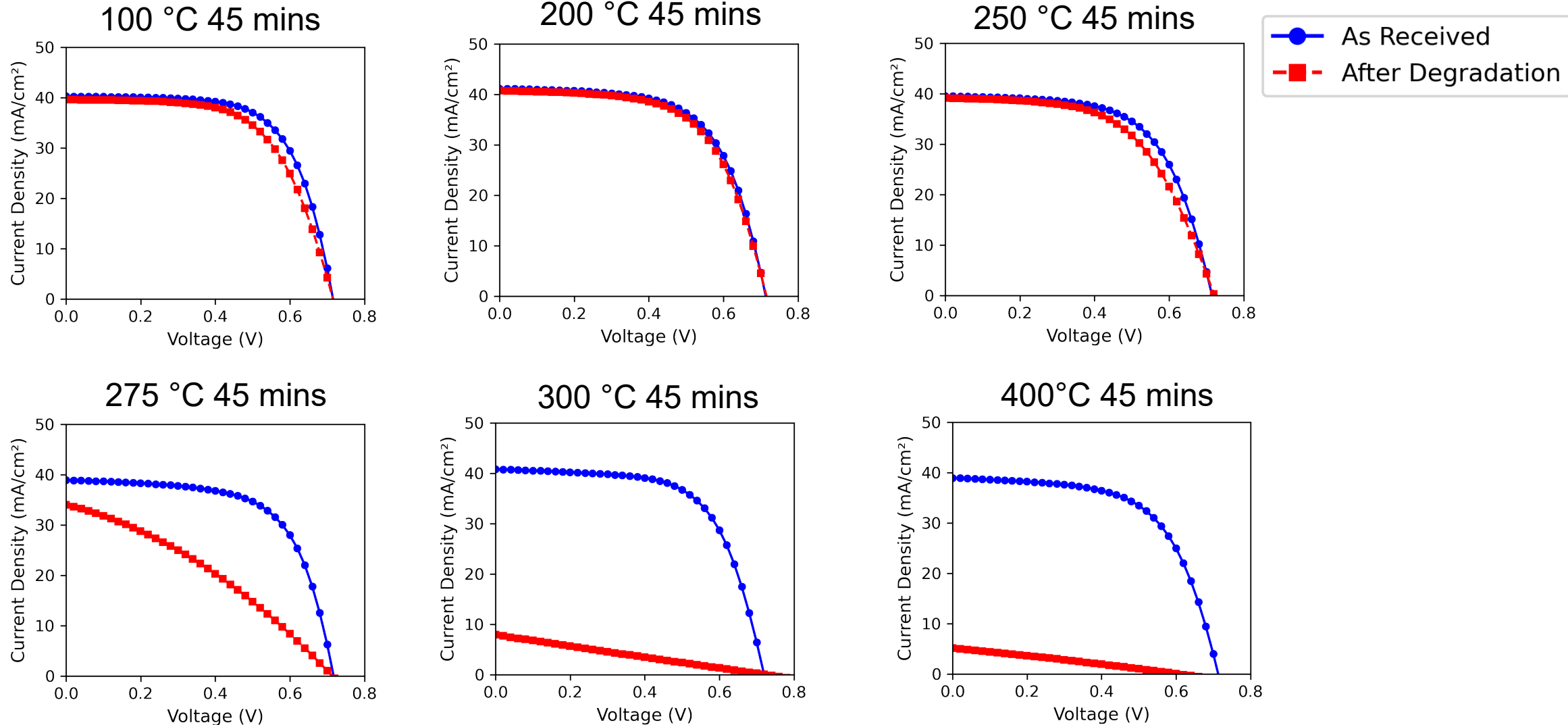
Literature support



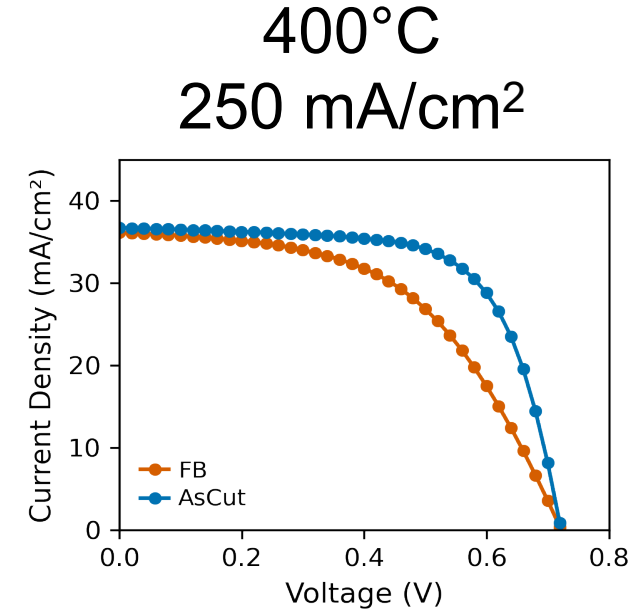
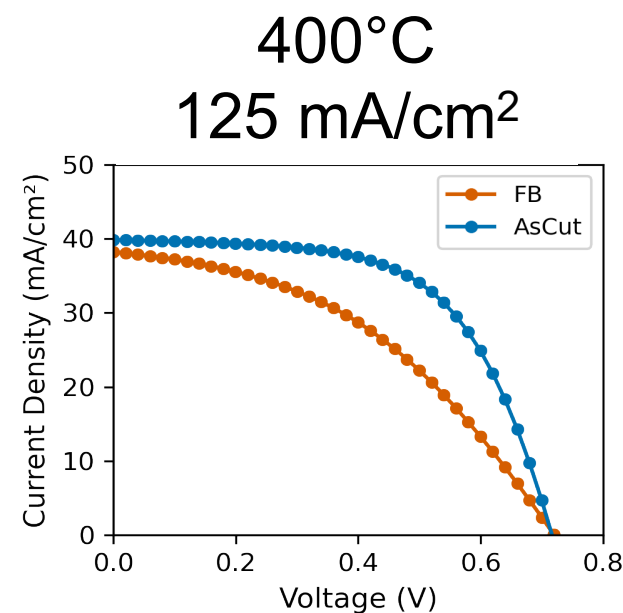
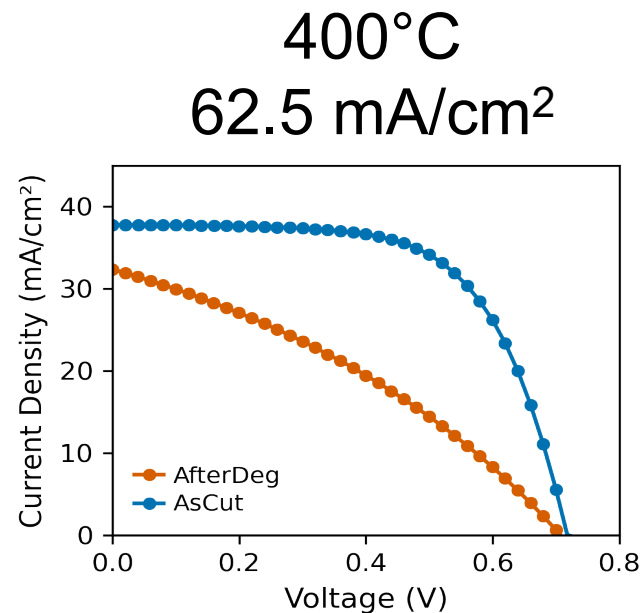
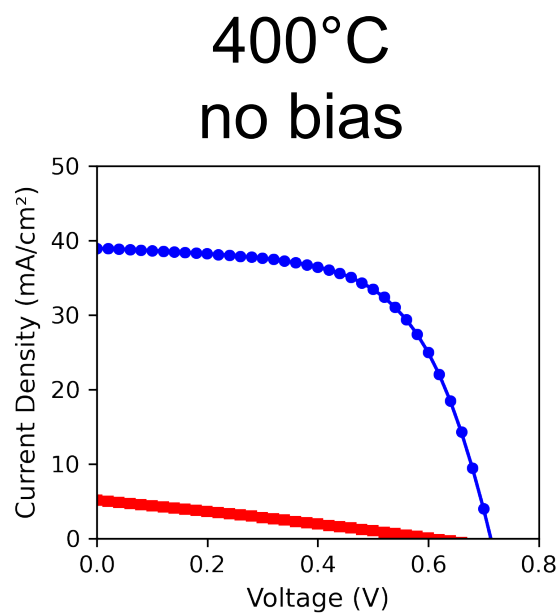
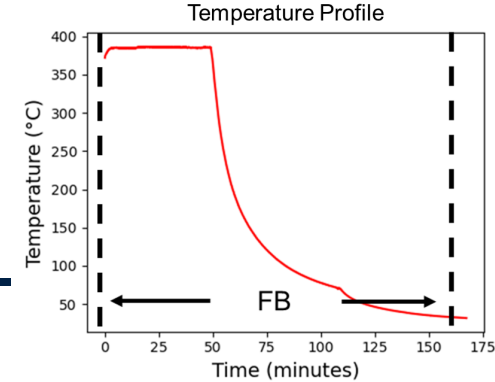
400°C was used to accelerate hydrogen-related degradation kinetics and enable clear measurement of the induced contact-resistance increase.

Liu et al., *Solar Energy Materials and Solar Cells*, 246, 111934 (2022).

Activation energy for LECO degradation



Forward bias improves IV stability at 400 °C



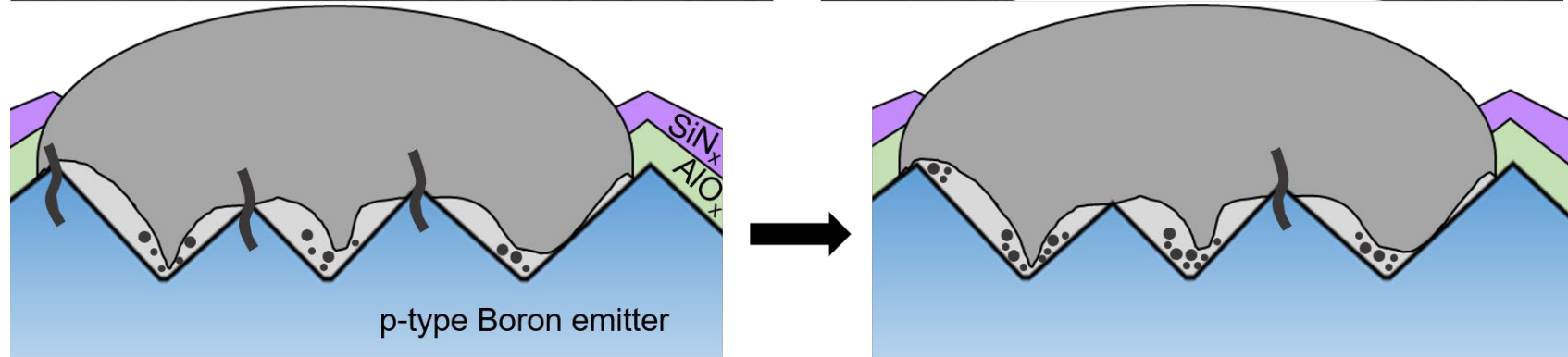
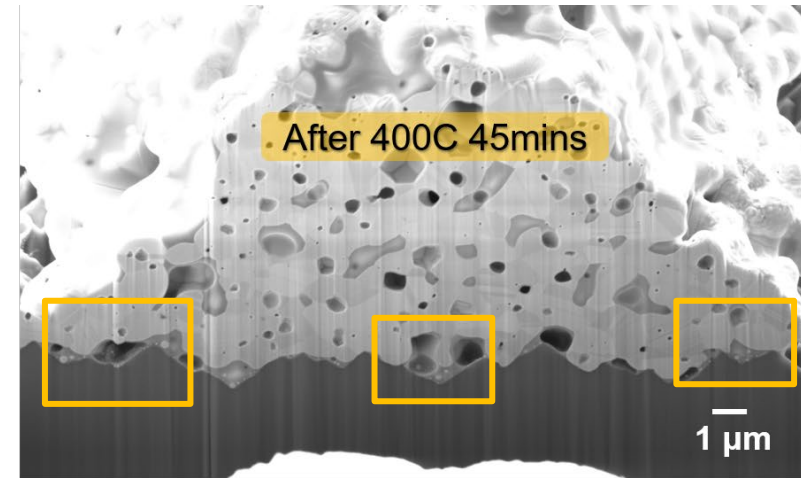
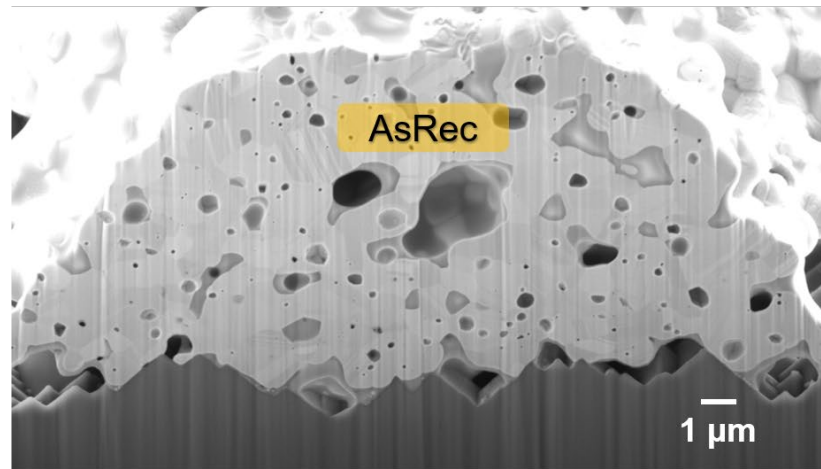
Condition	Jsc [mA/cm²]	Voc [mV]	FF [%]	Efficiency (eta) [%]	Condition	Jsc [mA/cm²]	Voc [mV]	FF [%]	Efficiency (eta) [%]	Condition	Jsc [mA/cm²]	Voc [mV]	FF [%]	Efficiency (eta) [%]
AsCut	37.81	719.36	63.41	17.25	AsCut	39.36	715.95	64.14	18.07	AsCut	38.38	721.57	67.16	18.6
FB 0.25A	32.37	707.75	34	7.79	FB 0.5A	38.23	717.12	43.9	12.04	FB 1A	36.18	722.34	51.72	13.52

- Increasing forward bias during 400 °C anneal progressively reduces IV degradation by stabilising series resistance.

Hypothesis 2: thermal instability of the LECO contact interface

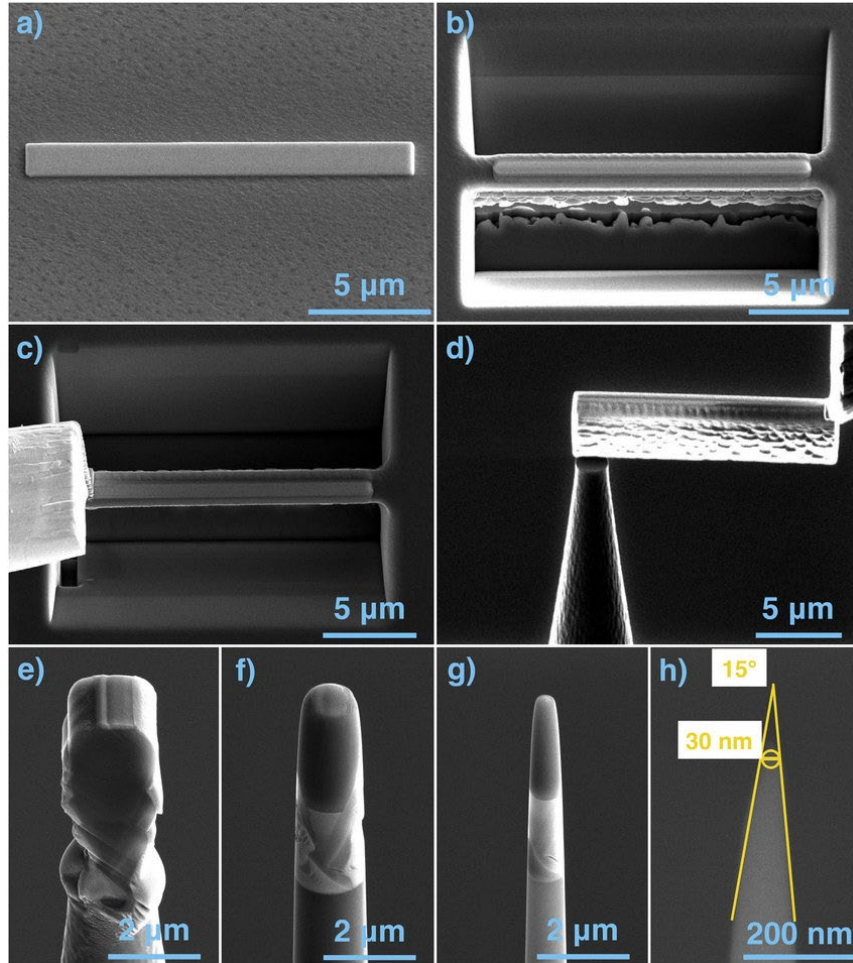
400°C dark anneal degradation

Bridges neck down and pinch off $\rightarrow$ Ag beads become rounder, more isolated $\rightarrow R_s \uparrow$.

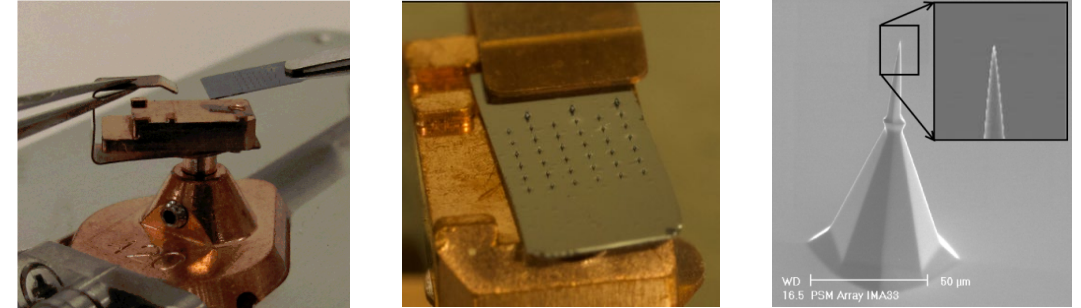


Atom Probe Sample Preparation Process

Conventional APT sample prep process



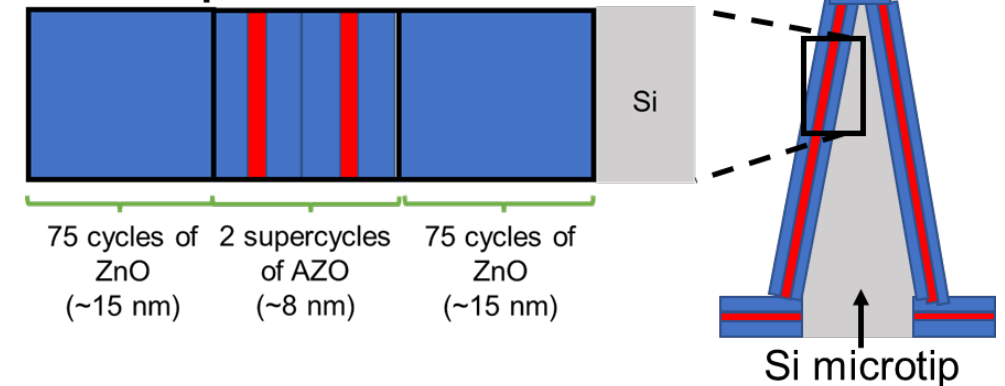
Pre-sharpened microtip coupon



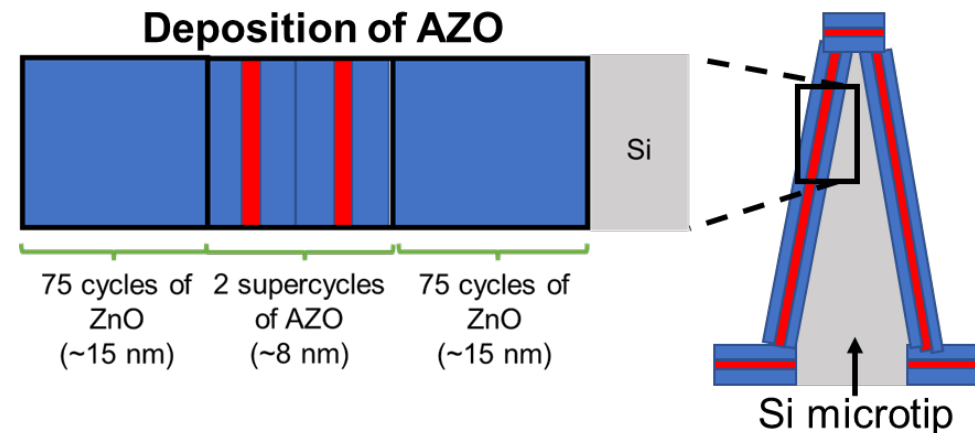
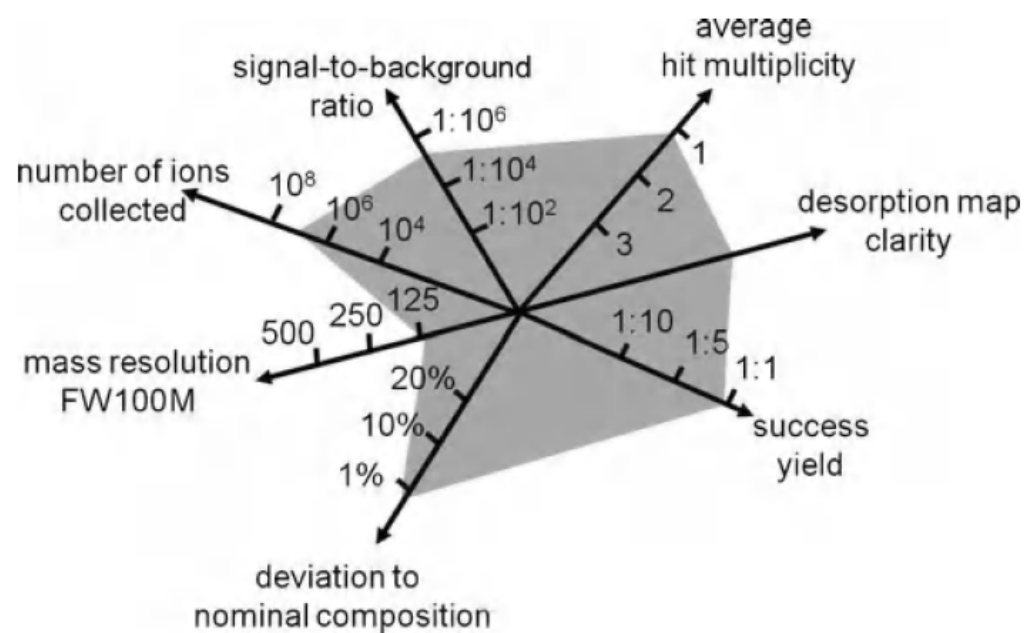
Chemical cleaning

- **Repeat 3×:** Apply 1% HF drop → DI water rinse → UV-ozone treatment.

Deposition of AZO



APT Parameter Optimisation



Need to optimise laser energy for:

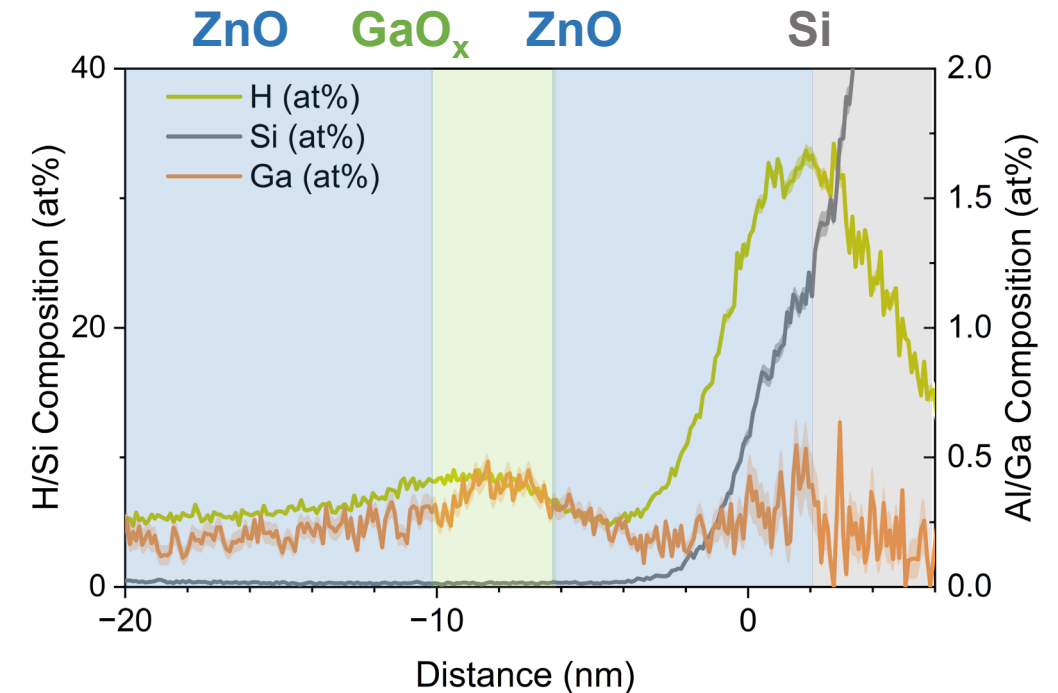
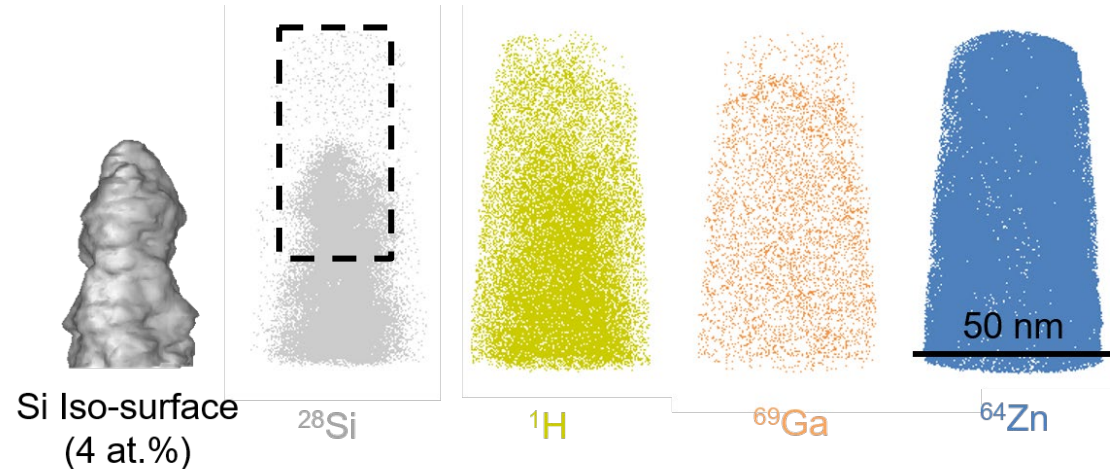
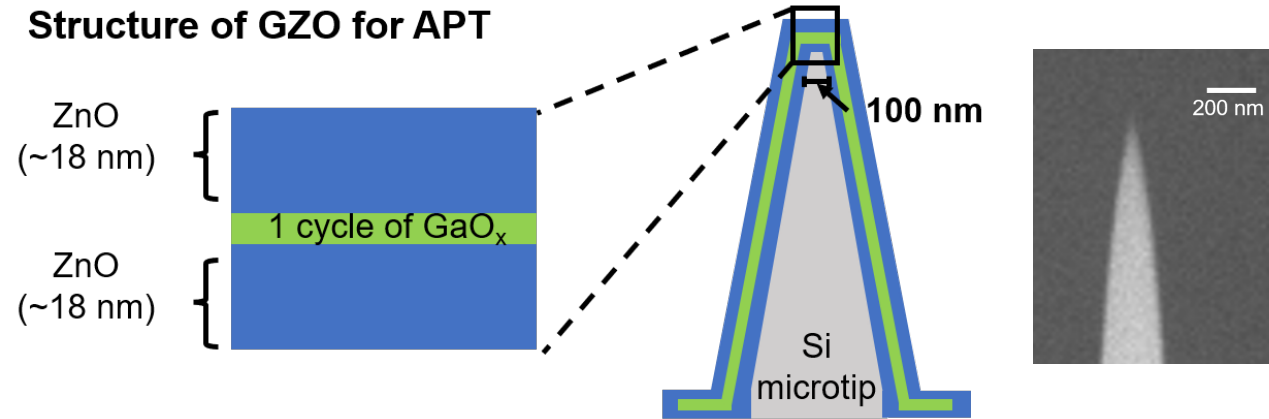
- Bulk ZnO matrix → CSR, multiplicity
- AlOx dopant → Al concentration distribution, Al detection

Need to optimise detection rate for:

- Bulk ZnO matrix → Multiples, CSR

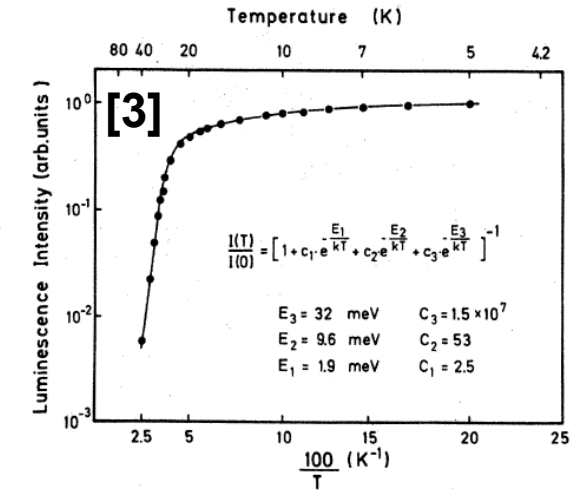
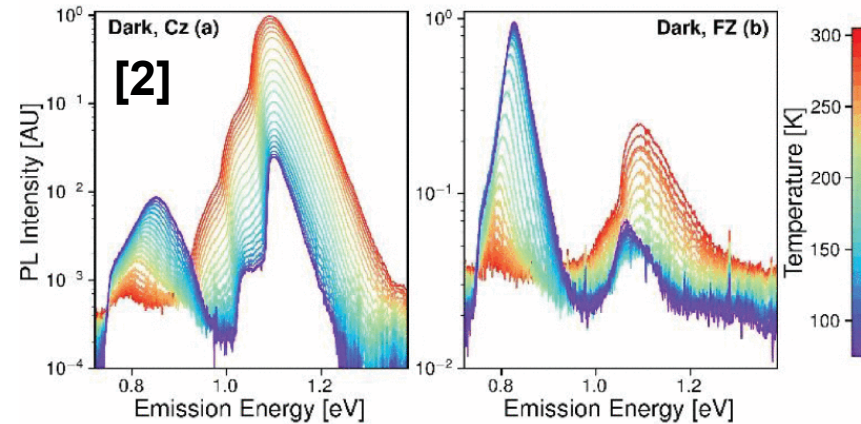
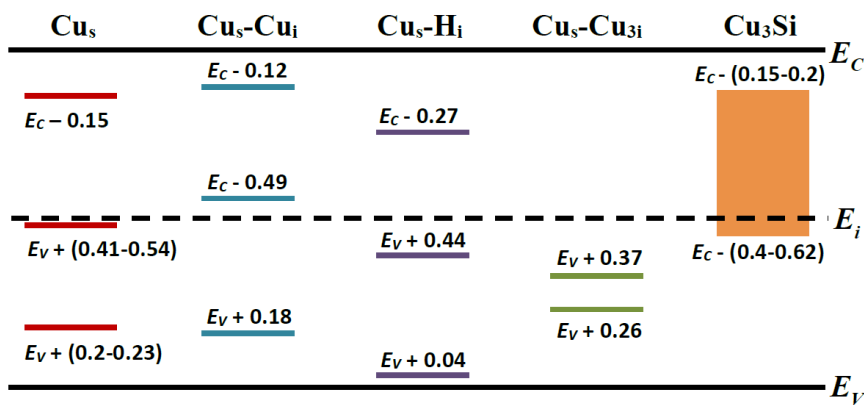
GZO extends the doped-ZnO comparison

Structure of GZO for APT



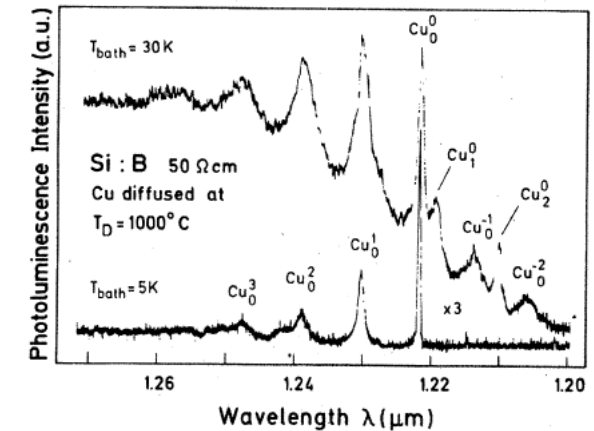
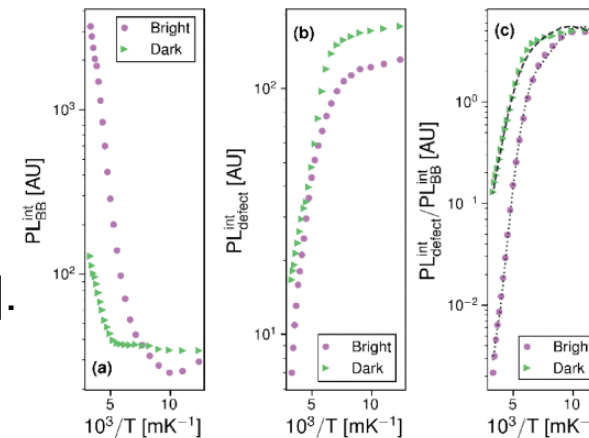
Copper Defects in Silicon

Cu defect energy levels in Si [1]:



- Temperature-dependent micro PL [2].
- Temperature and injection-dependent lifetime spectroscopy [1] – need to etch metal off.

$\text{Cu}_s\text{Cu}_{3i}$ complex often associated with an intense zero-phonon photoluminescence (PL) emission at 1.014 eV [3].

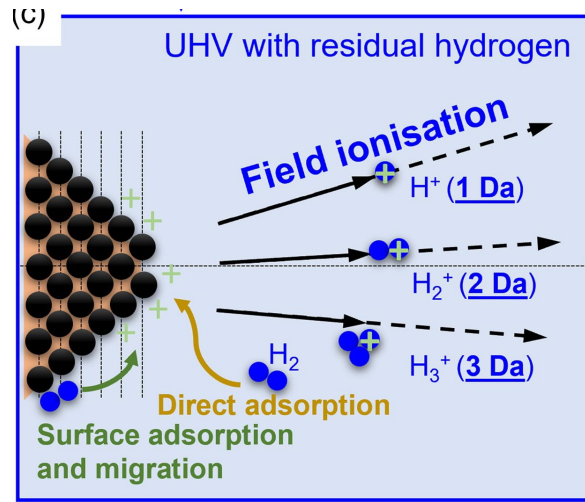


[1] J. Colwell, PhD Thesis, UNSW, 2018

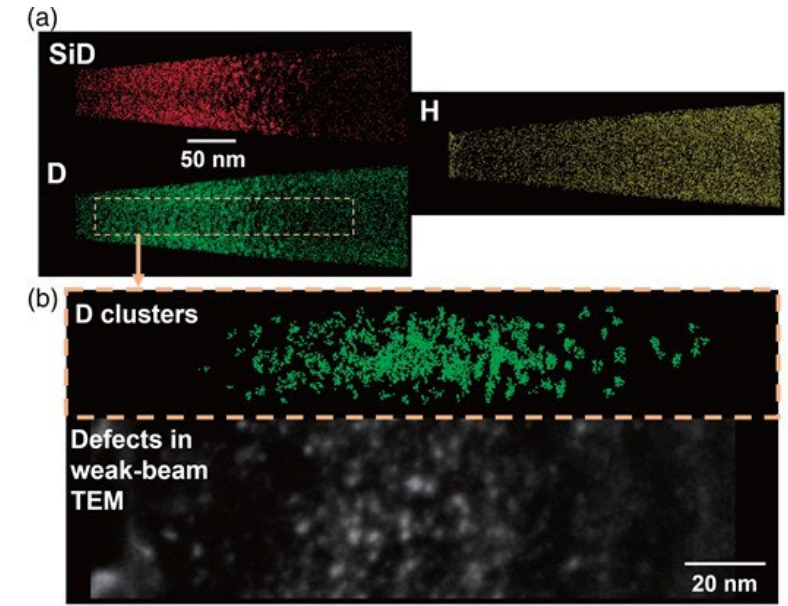
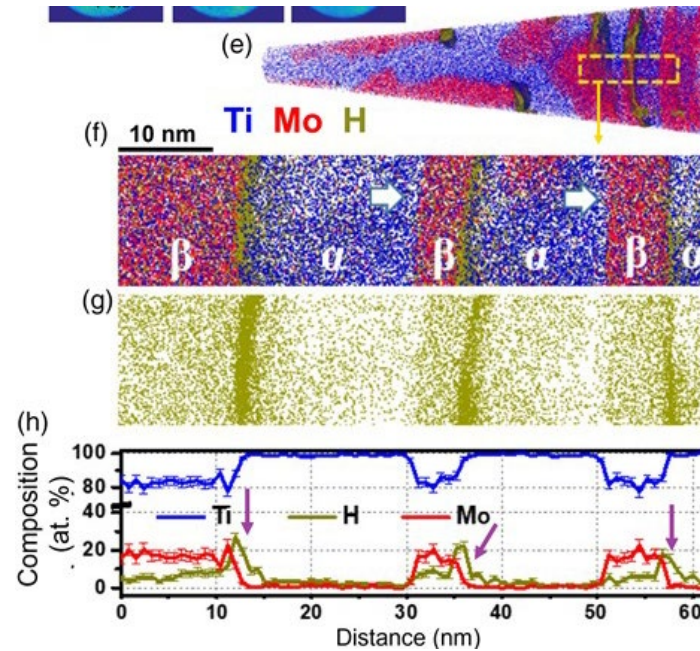
[2] R. L. Chin et al., "Insights into Bulk Defects in n-type Monocrystalline Silicon Wafers via Temperature-Dependent Micro-Photoluminescence Spectroscopy," WCPEC, 2018.

[3] J. Weber, H. Bauch & R. Sauer, Phys. Rev. B 25, 7688–7699 (1982).

Challenges of Hydrogen Quantification by Atom Probe Tomography

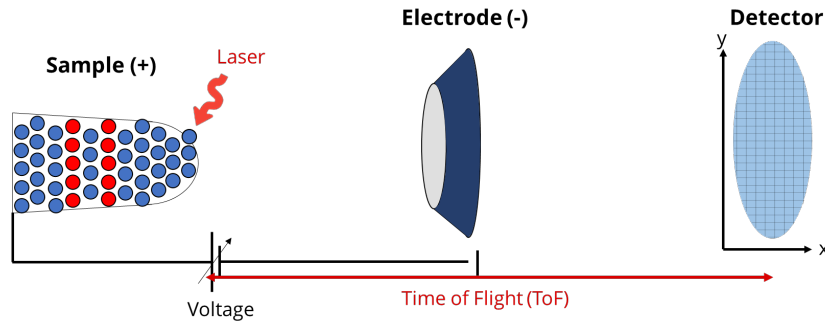
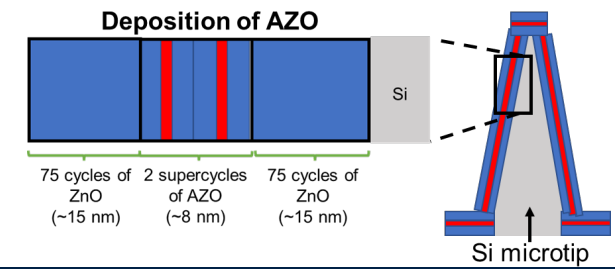


- Residual H from stainless steel chamber walls (AISI 304/316L).
- H supply to the tip:
 - Direct adsorption on the apex.
 - Shank adsorption + surface diffusion.



APT studies have shown that background hydrogen often appears uniformly distributed, whereas specimen-derived hydrogen can show clustering or segregation.

Frequency Cycling to Distinguish Contaminant and Sample Hydrogen



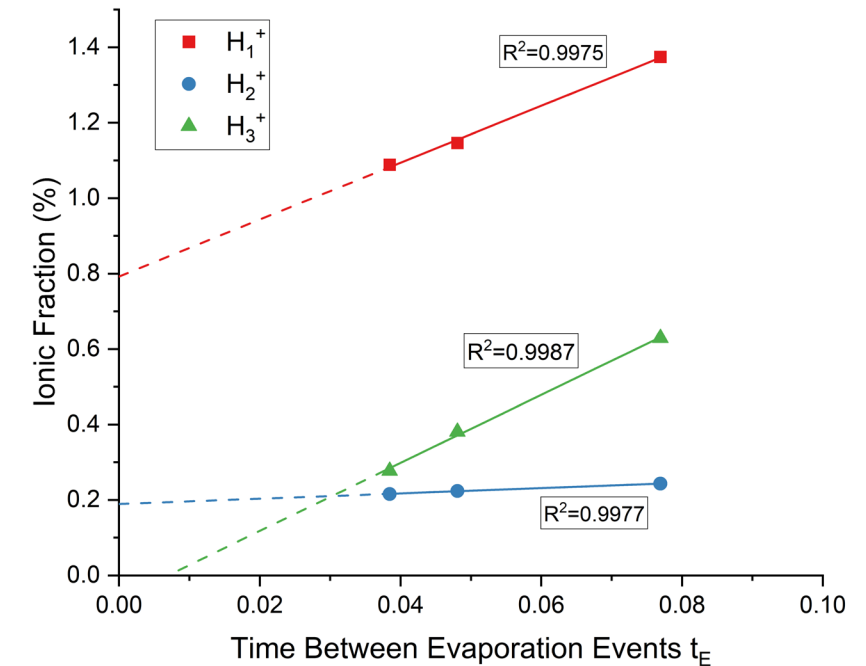
time between evaporation events

$$t_E = \frac{1}{f_{\text{pulse}} r_{\text{det}} \zeta}$$

f_{pulse} : pulse frequency
 r_{det} : detection rate
 ζ : detector efficiency

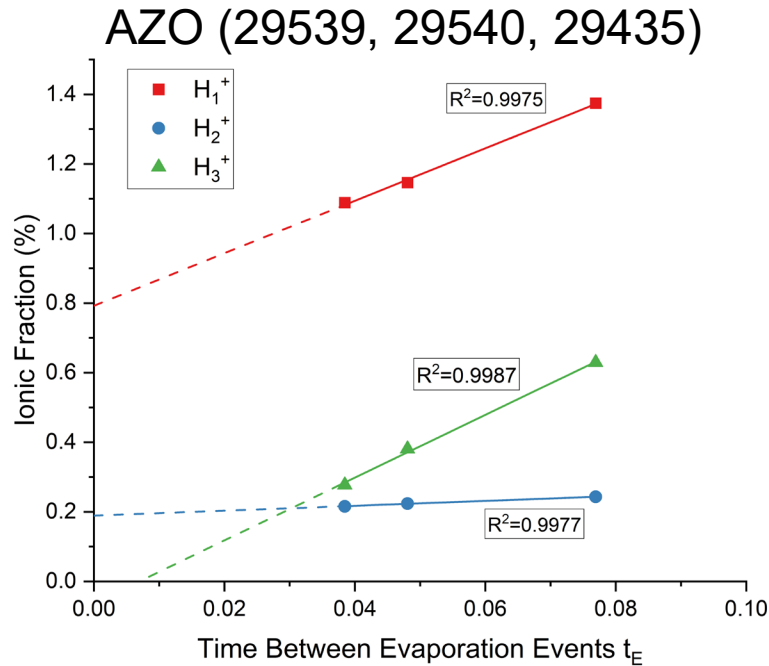
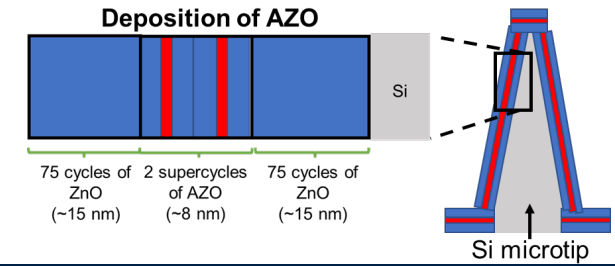
- Contaminant H is time-dependent.
- Higher pulse frequency $\rightarrow$ shorter $t_E \rightarrow$ less contaminant H.
- Extrapolate to $t_E = 0$ to estimate the real sample hydrogen.

AZO (29539, 29540, 29435)



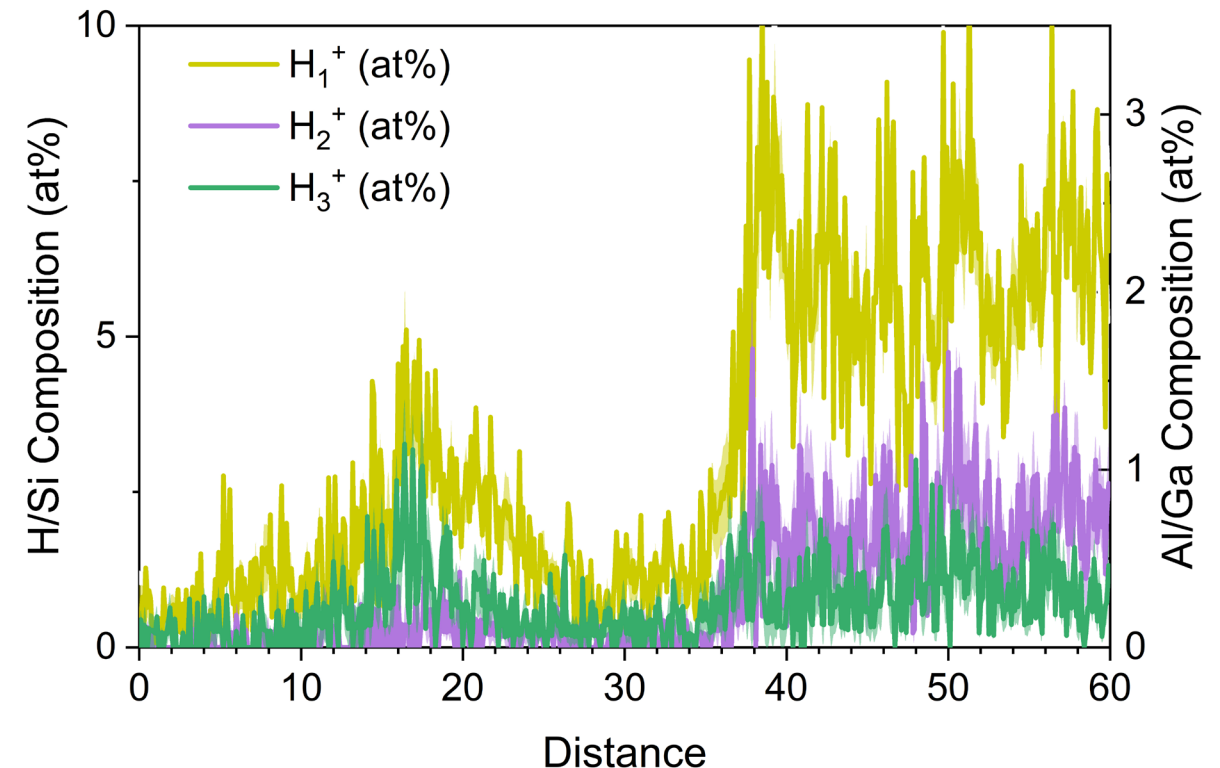
- H⁺ and H₂⁺ are more likely to contain both contaminant and sample hydrogen.
- H₃⁺ is more likely dominated by contaminant hydrogen.

Hydrogen Contents by Ionic Species



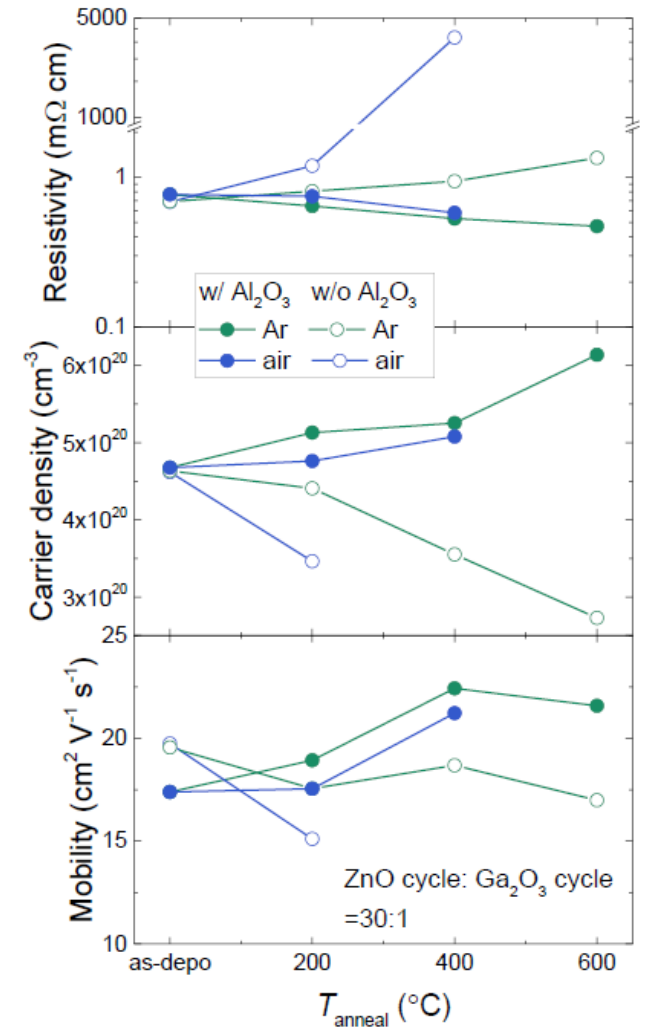
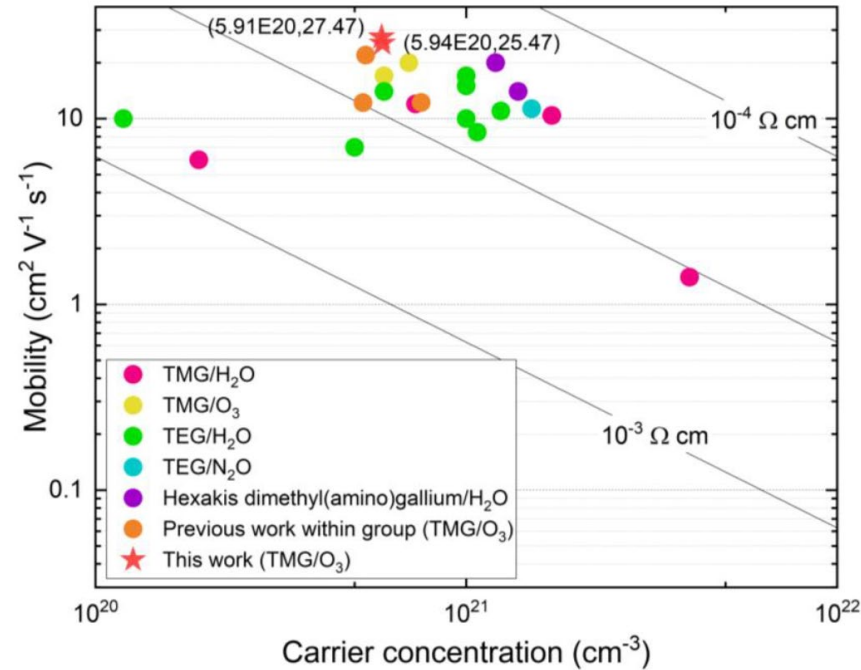
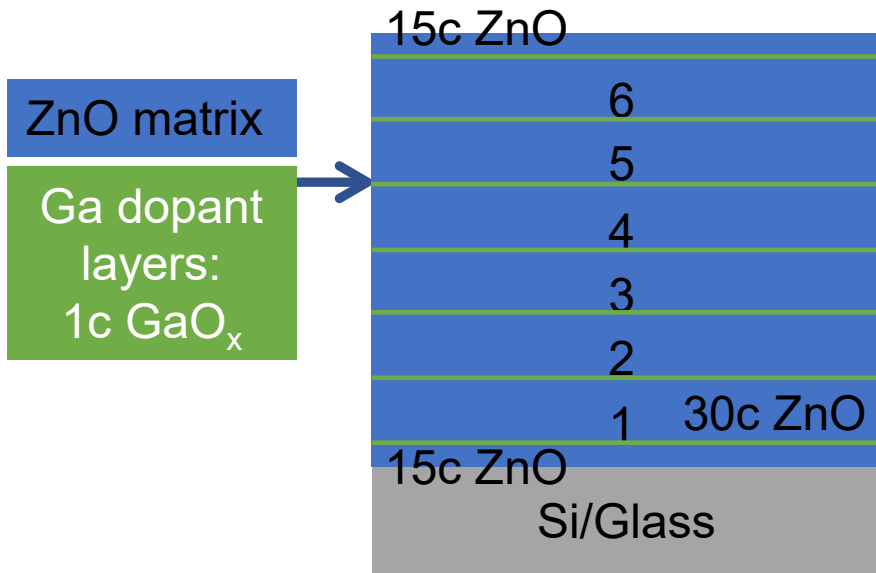
- H^+ and H_2^+ are more likely to contain both contaminant and sample hydrogen.
- H_3^+ is more likely dominated by contaminant hydrogen.

As-deposited

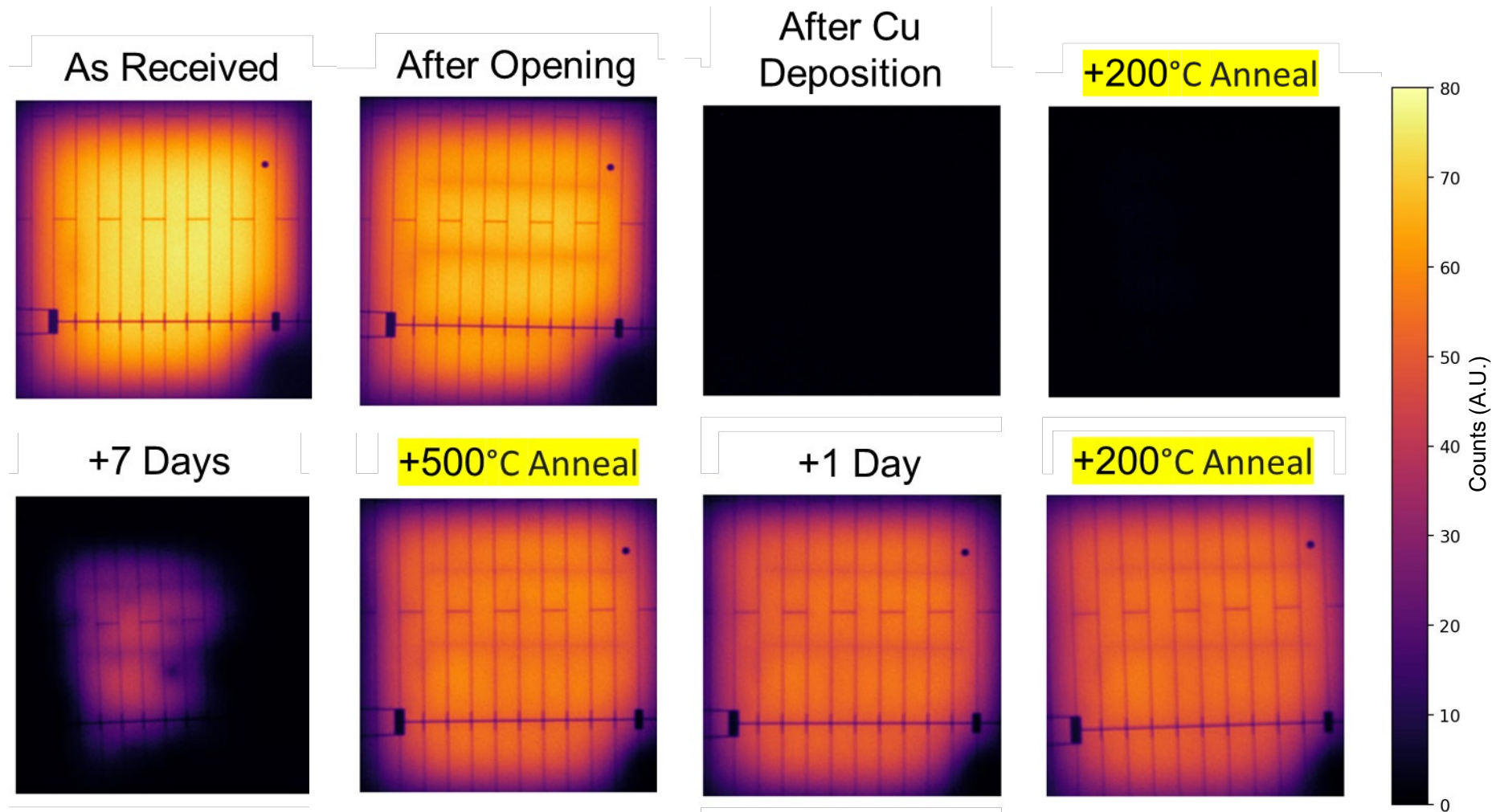


- H^+ peak at AlO_x and Si/ZnO interface could be real!

Indium-free Transparent Conducting Oxide - Gallium-doped Zinc Oxide (GZO)



Anneal Sequence: 200°C – 500°C – 200°C



Cu

