Understanding CdSe in CdTe Devices

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Loughborough PV Research

Loughborough University

Housed in the Centre for Renewable Energy Systems Technology (CREST)

- CREST: 60 Staff, students
- 30 funded programs each up to £3M

Increasing Efficiencies

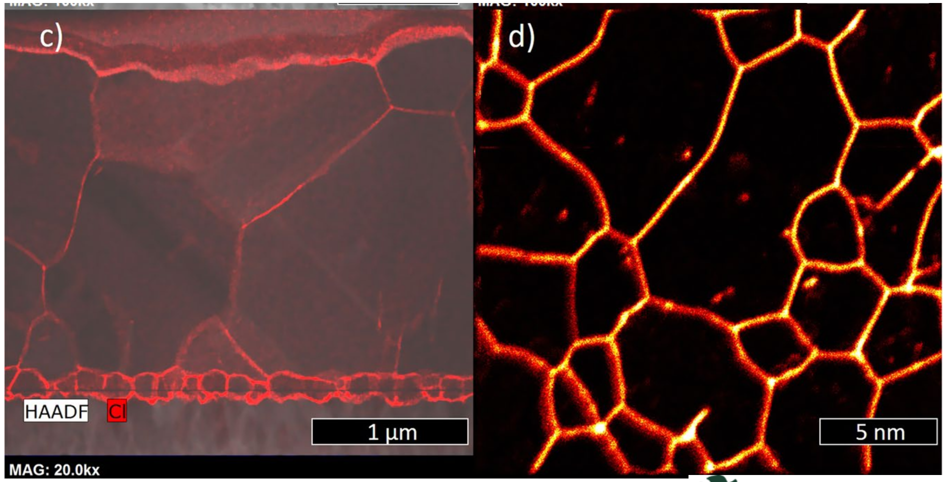
- Doped, stable front emitter
- Enhanced group V doping and activation
- Optimized back contact / buffer
  - Back passivation

Advanced Device

- Bifacial designs
- Durable anti-reflection / anti-Soiling coatings
- Fundamental understand via characterization and DFT simulation

PV Team

- 5 Academics
- 5 Professional Research Associates
- 12+ Ph.D. Students



Hatton et. Al. Nature Comm. 12, no. 1 (2021)

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Outline

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- Xe FIB, EBSD cross section technique
- Devices with **CdSeTe** alloy film deposition
- Devices with **CdSe**
  - $CdCl_2$ and diffusion
- Cathodoluminescence

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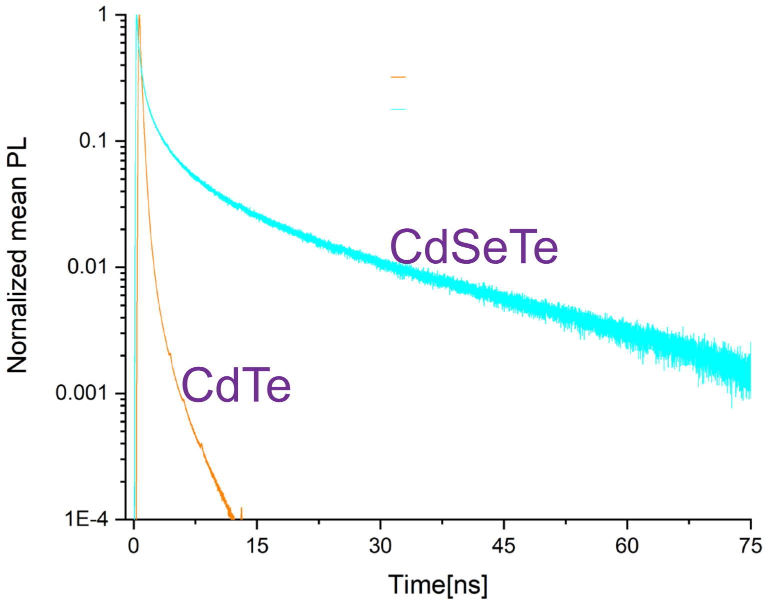
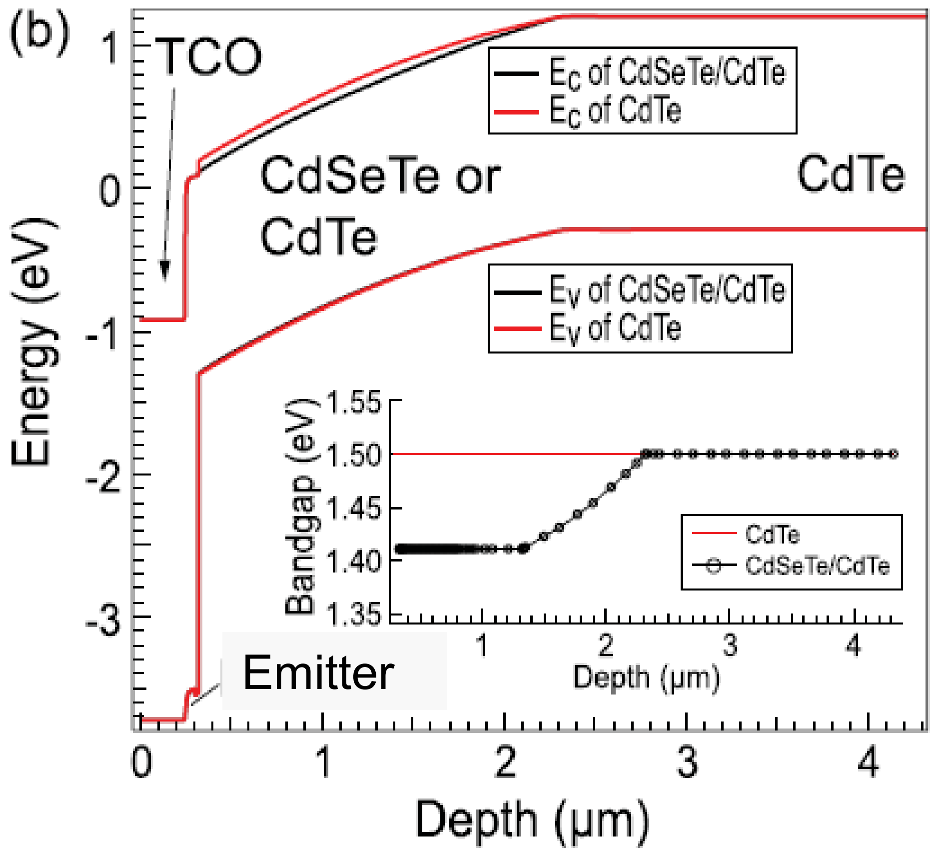
CdSeTe / CdTe Devices

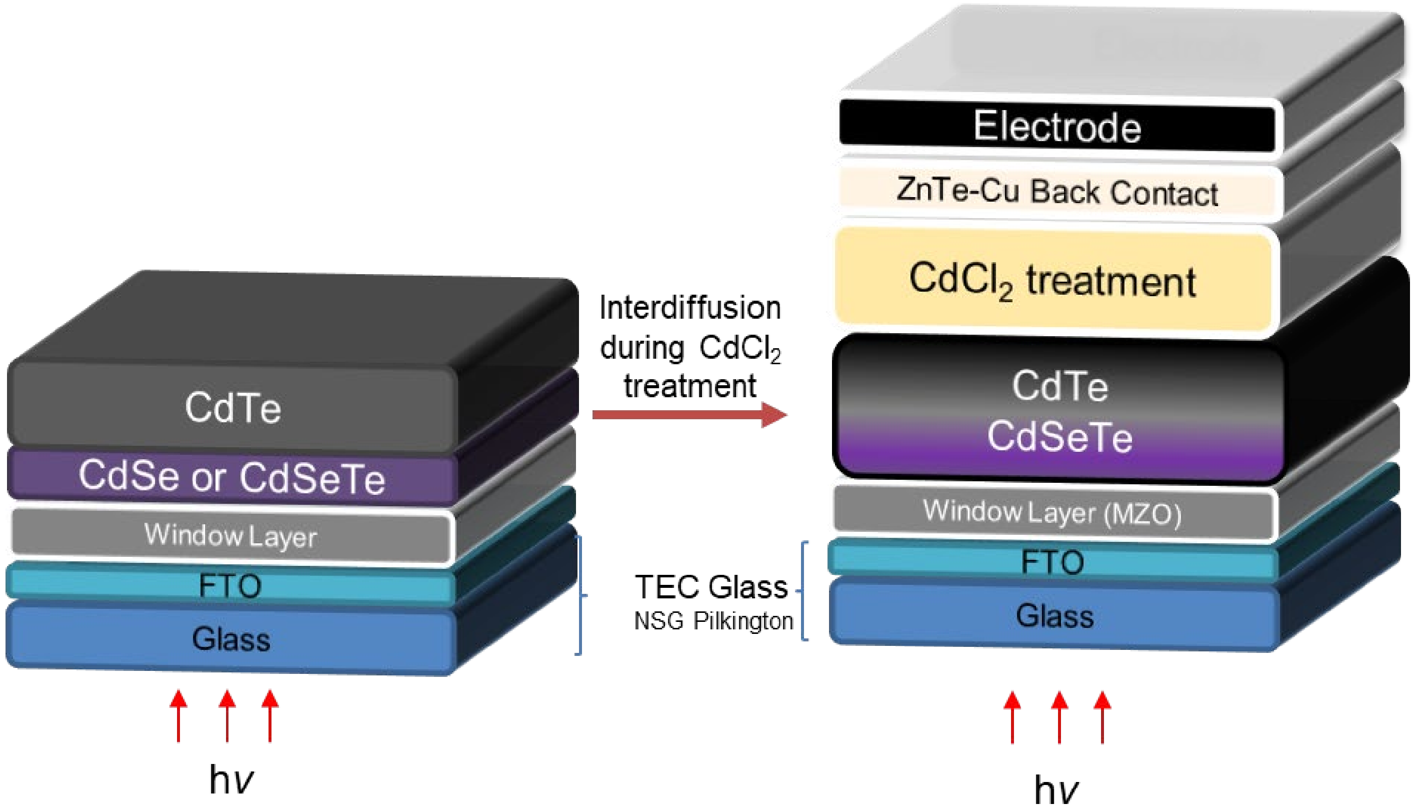
- Bandgap grading
  - CdSeTe alloy can be have Eg between 1.38 eV – 1.5 eV
- Passivates defects in bulk
  - Shown through improved CL intensity [1]
- Increases carrier lifetime





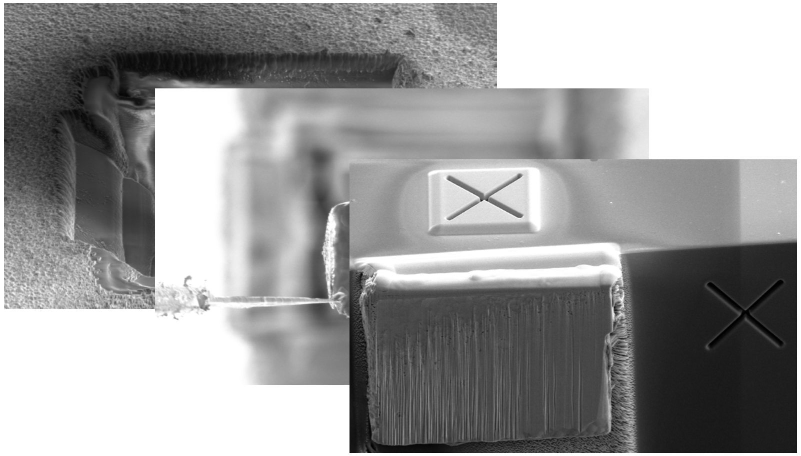
1: Nature Energy 4, no. 6 (2019)

Introducing Se in CdTe solar cells

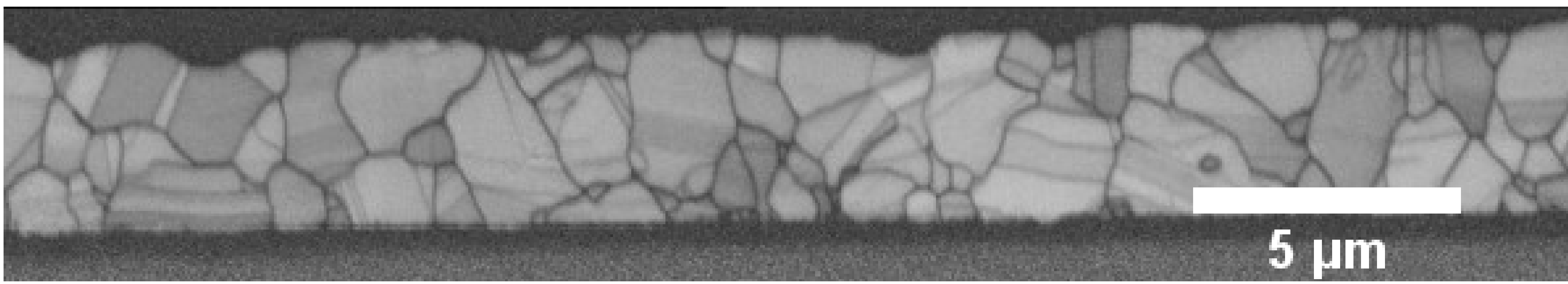


Either CdSe or CdSeTe deposited followed by $CdCl_2$ used to form absorbers

Characterization: Advanced EBSD



- Ion mill chunk, lift out onto a Si wafer
- 50nm thick, fiducial markers for alignment
- Xe FIB
  - Rapid, minimized FIB damage



EBSD: 350 micron wide area (continues off slide)

~ 2 hours from cell sample to images and EBSD analysis
Xe FIB is enabling

Devices with CdSeTe Film Deposition (then CdCl2)

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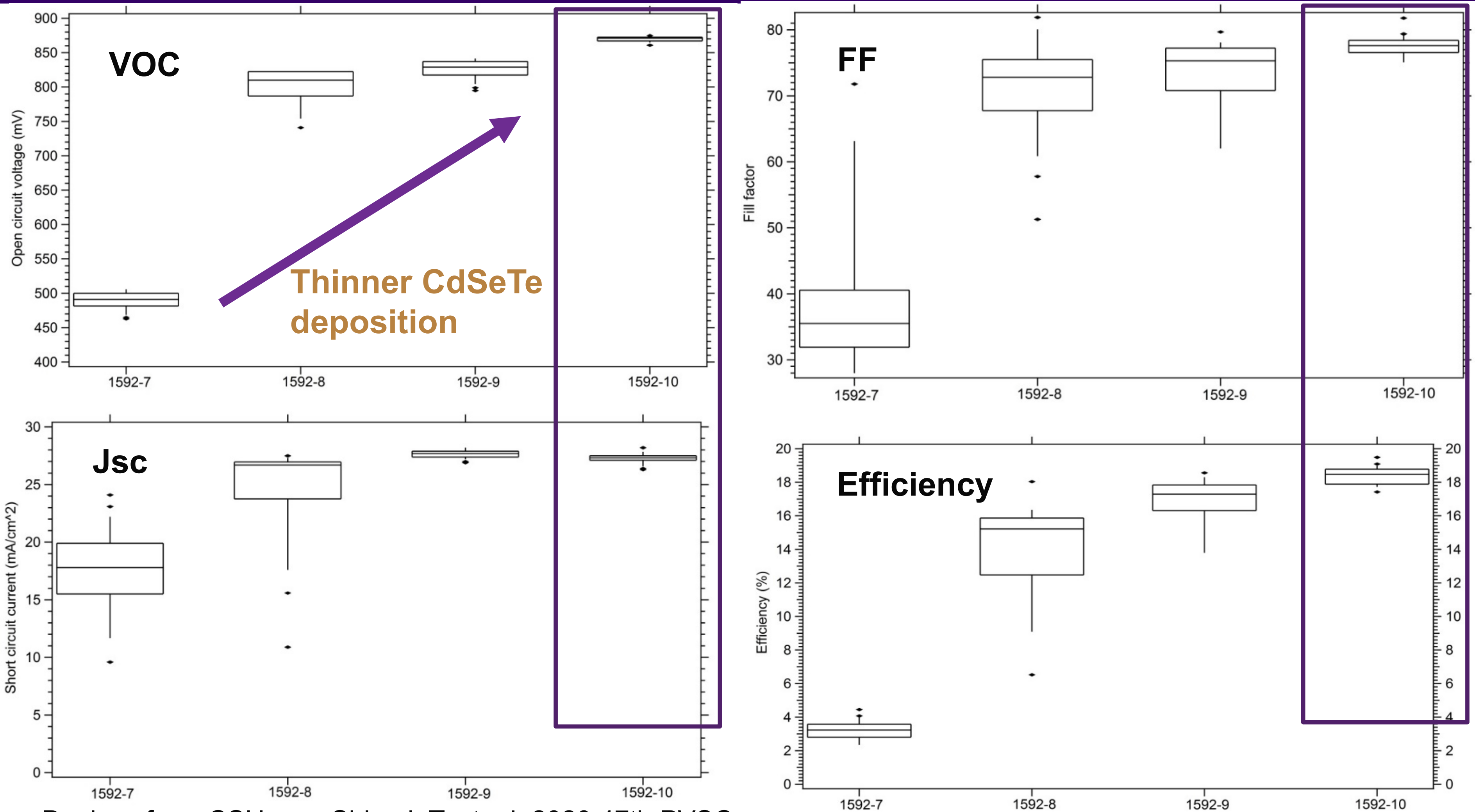

Devices from CSU, see Shimpi, T. et. al. 2020 47th PVSC

Performance sensitive to CdSeTe
CdSeTe devices without CdTe are poor

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Absorber from CdSeTe / CdTe films (post $CdCl_2$)

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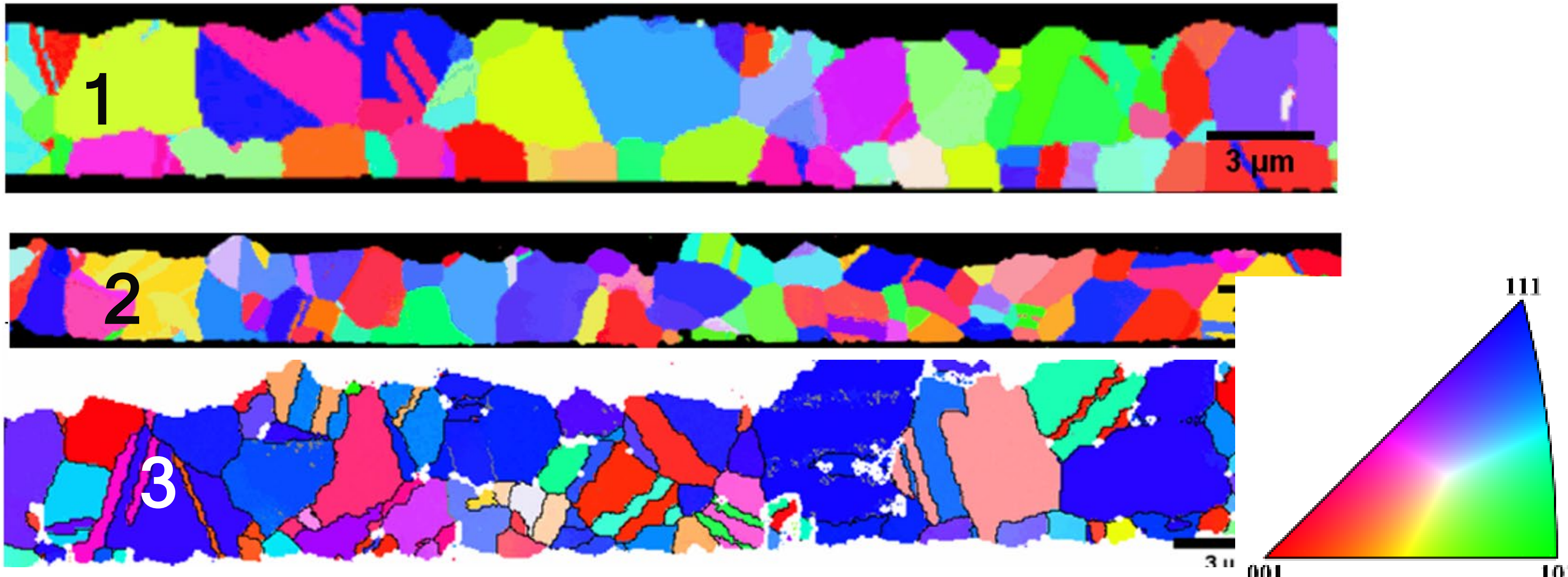

Device	PCE (%)	Voc [mV]	Jsc	FF [%]	Condition
1 (1592-10)	18.76	873	27.4	78.5	Thin CdSeTe, yielded larger mixed alloy layer, random texture
2 (1592-9)	17.22	828	27.4	75.8	Thicker CdSeTe, thinner CdTe
3 (1673-2)	17.33	851	26.9	75.7	Thinner CdSeTe, Insufficient CdCl2

111 texture orientation seen with insufficient $CdCl_2$ treatment, lower performance

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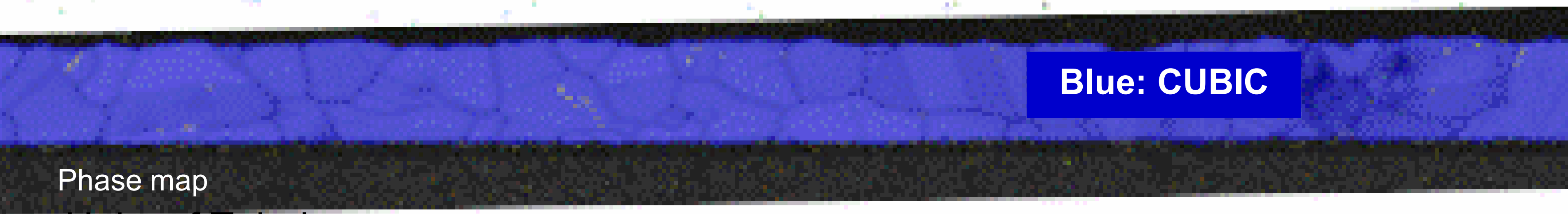
Absorber from CdSe films

Device: 120 nm CdSe (evaporated)/CdTe then $CdCl_2$ treatment



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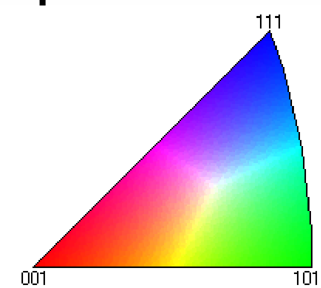
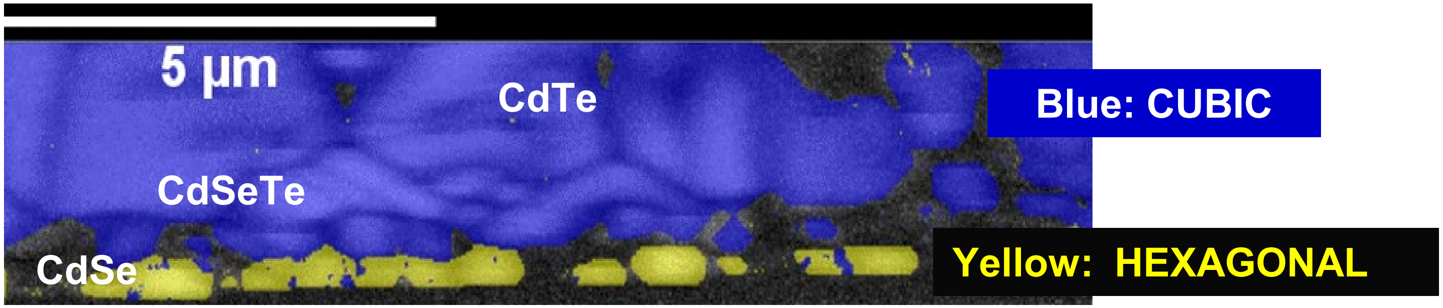
CdSe thickness (nm)	Estimate CdSeTe Eg	Eff. (η%)	Voc	Jsc	FF (%)
120	1.42	<u>16.1</u>	808	28.2	70.6

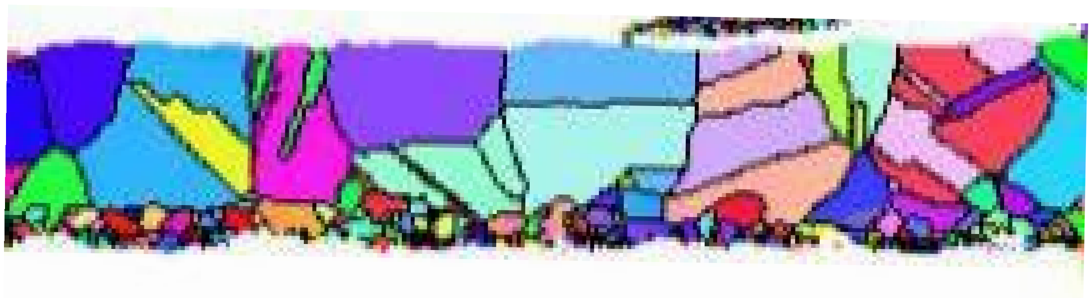


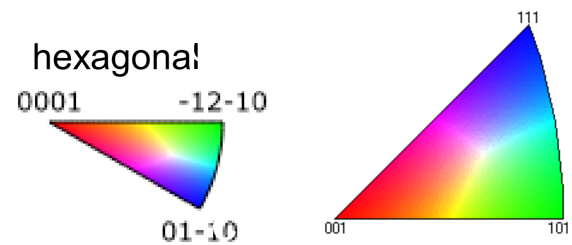
- All CdSe consumed during $CdCl_2$, Mixed alloy CdSeTe formed
- Generally random texture
- All cubic phase
- Similar to CdSeTe film dep

Absorber from CdSe films

Device: 400 nm CdSe (evaporated)/CdTe, then $CdCl_2$ treatment







CdSe thickness (nm)	Estimate CdSeTe Eg	Eff. (η%)	Voc	Jsc	FF (%)
400	1.39	<u>6.1</u>	784	11.7	66

- Hexagonal CdSe remaining
- **Poor efficiency : 6.1 %, with low Jsc**

Insufficient $CdCl_2$ damaging with CdSe films
Rapid EBSD can help optimize chloride process

Absorber from CdSe films

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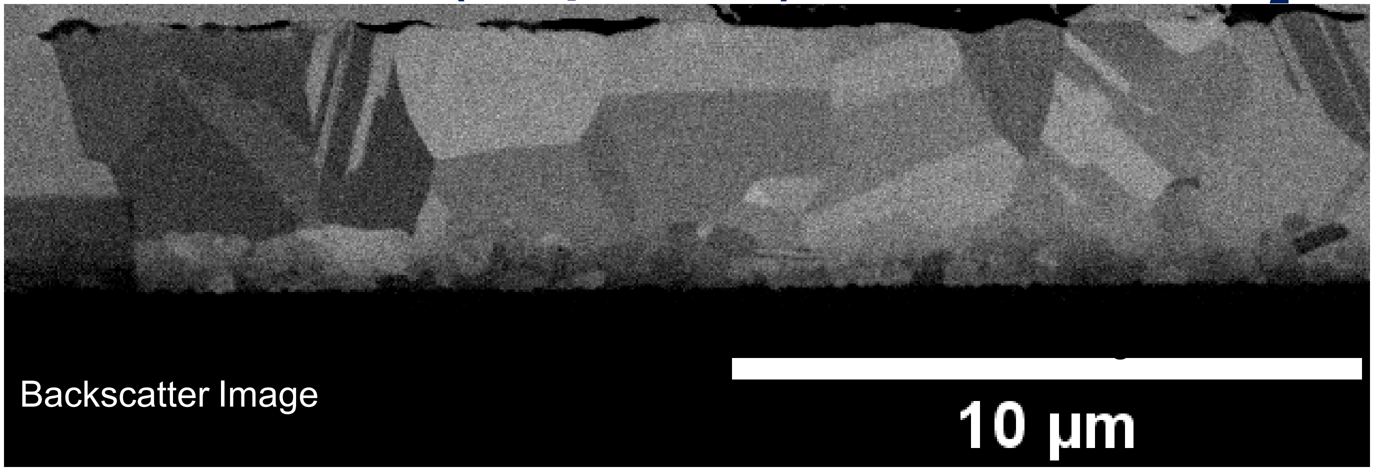
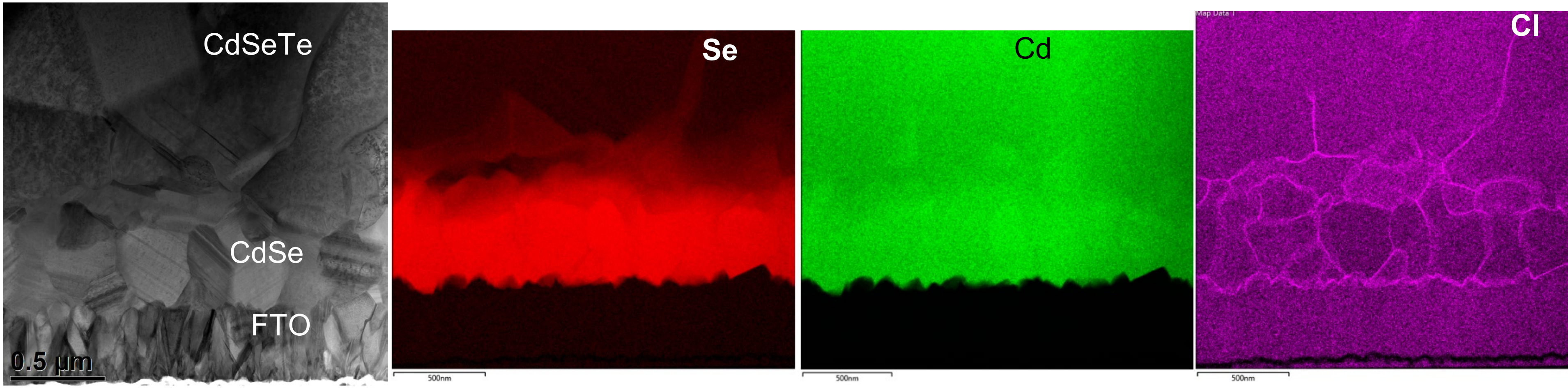
Device: 400 nm CdSe (evaporated)/CdTe, then $CdCl_2$ treatment





Chlorine present in the CdSe (and CdSeTe) grain boundaries

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EQE CdSe / CdSeTe device

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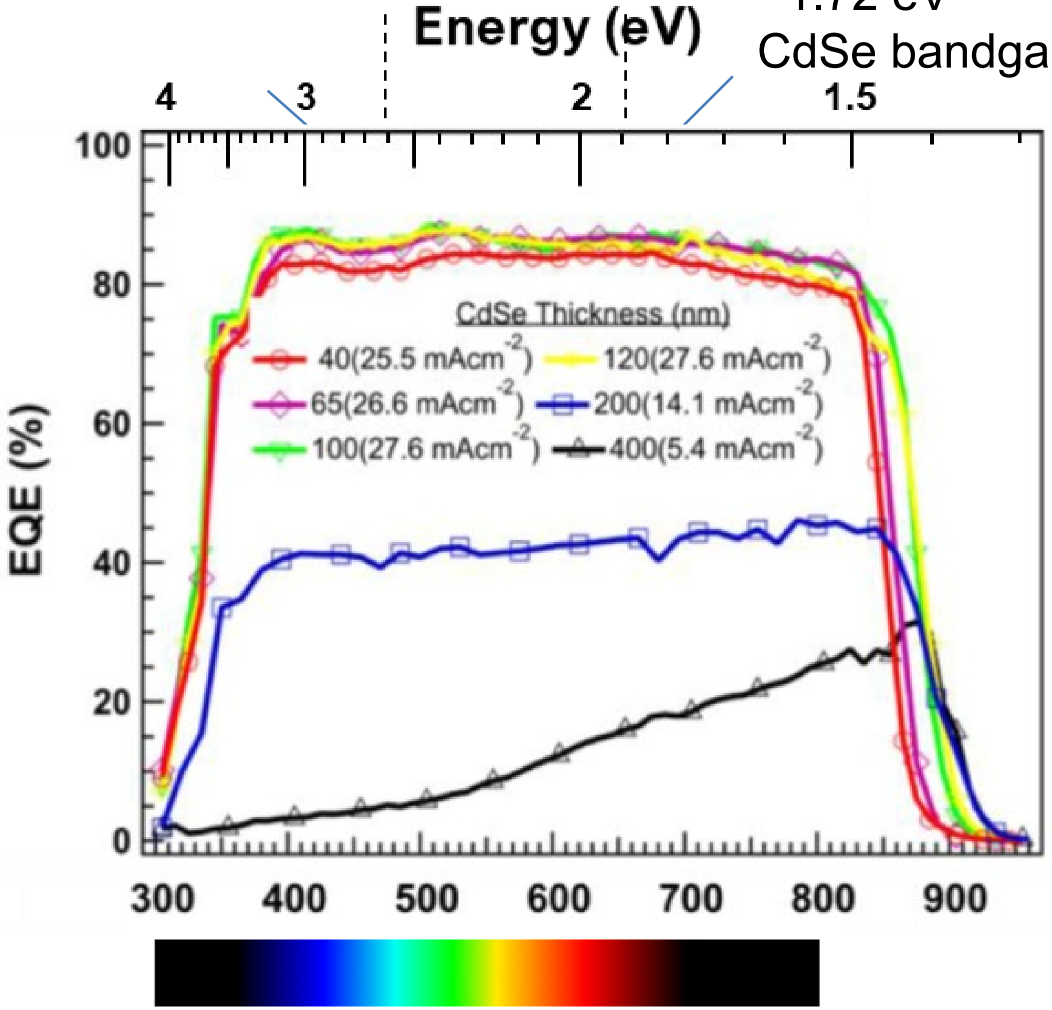
CdSe present at the front of the device causes:

- parasitic absorption (optical effect), Eg: 1.74eV

- CdSe is n-type so there is the electrical effect of moving the p-n junction deeper into the device – 'buried junction' (electrical effect)

- Hexagonal structure of CdSe leads to poor carrier transport across cubic CdSeTe

~1.72 eV – CdSe bandgap



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Cathodoluminescence of CdSeTe: Se and Grain Boundaries

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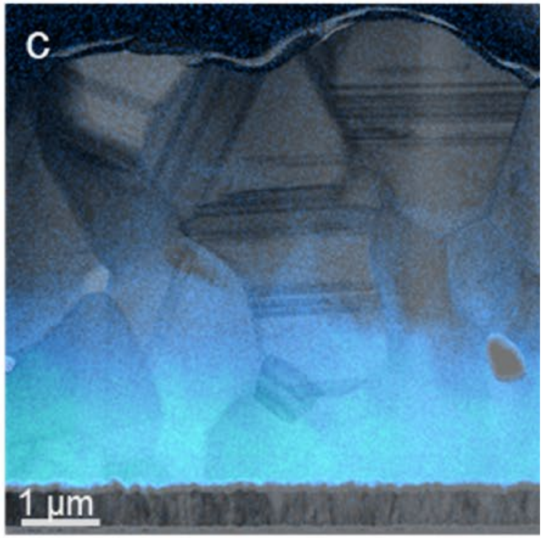
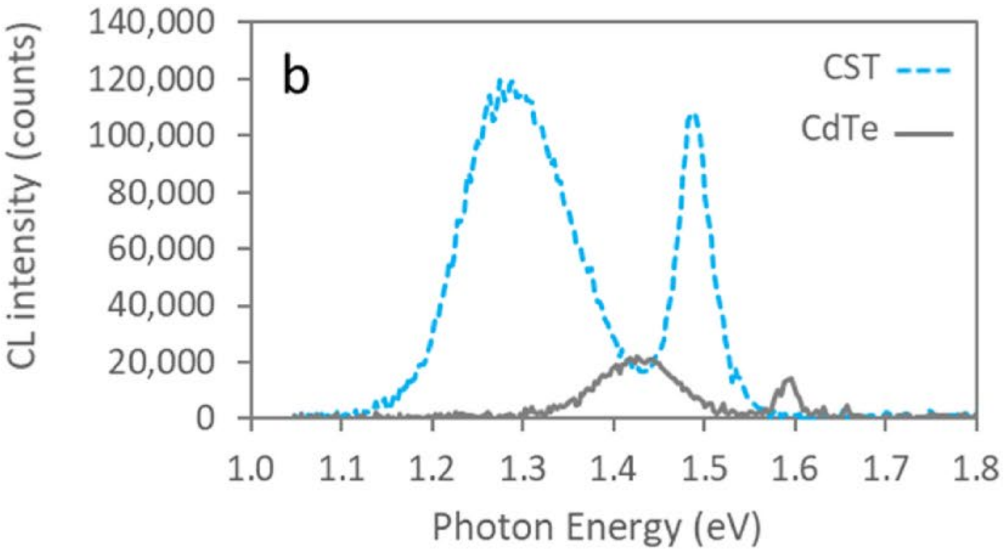


Fiducia, et. al., Solar Energy Materials and Solar Cells Vol. 238, 2022.



Grain boundary CL measurements

Low temperature CL along grain boundaries

CdSeTe: Higher CL than CdTe

CL measurements: Se passivates grain boundaries

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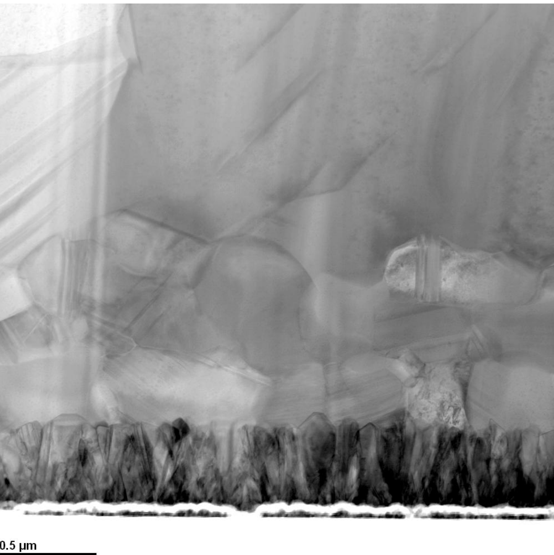
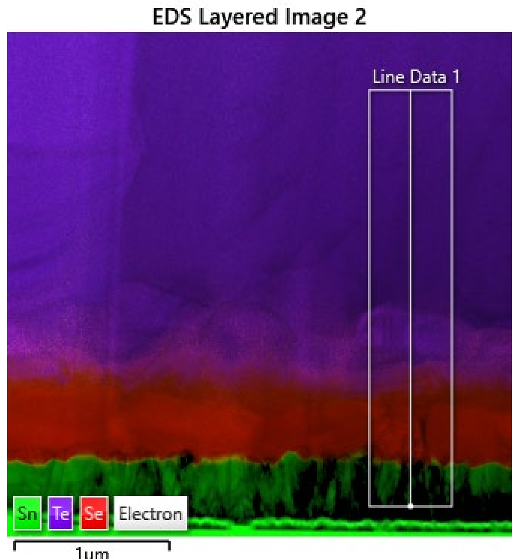
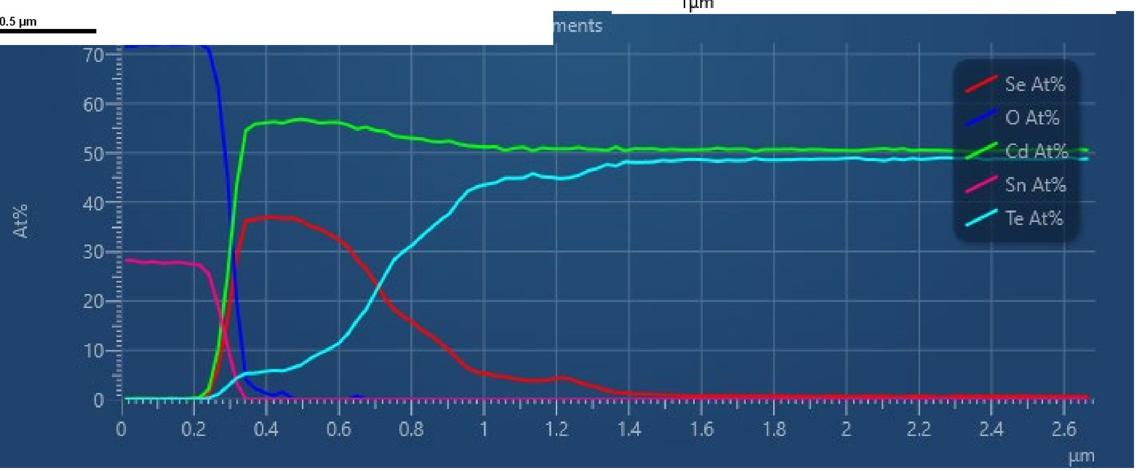
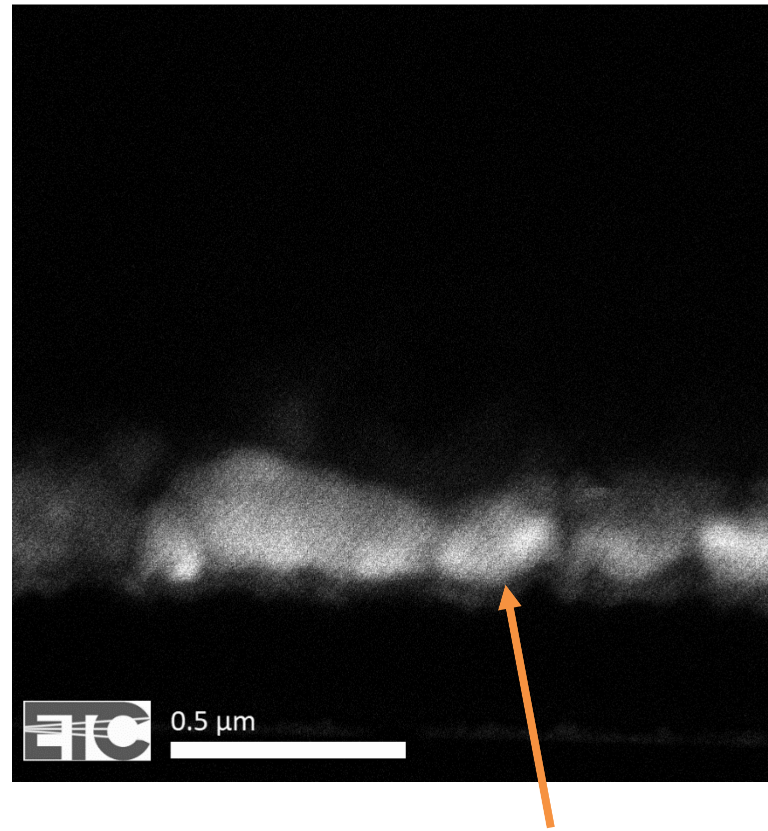
Cathodoluminescence of treated CdSe

Device: 400 nm CdSe (evaporated)/CdTe, then $CdCl_2$ treatment









~50 times more intense CL signal in hexagonal CdSe region that has not been fully consumed than CdTe

CL of UNTREATED CdSeTe / CdTe devices

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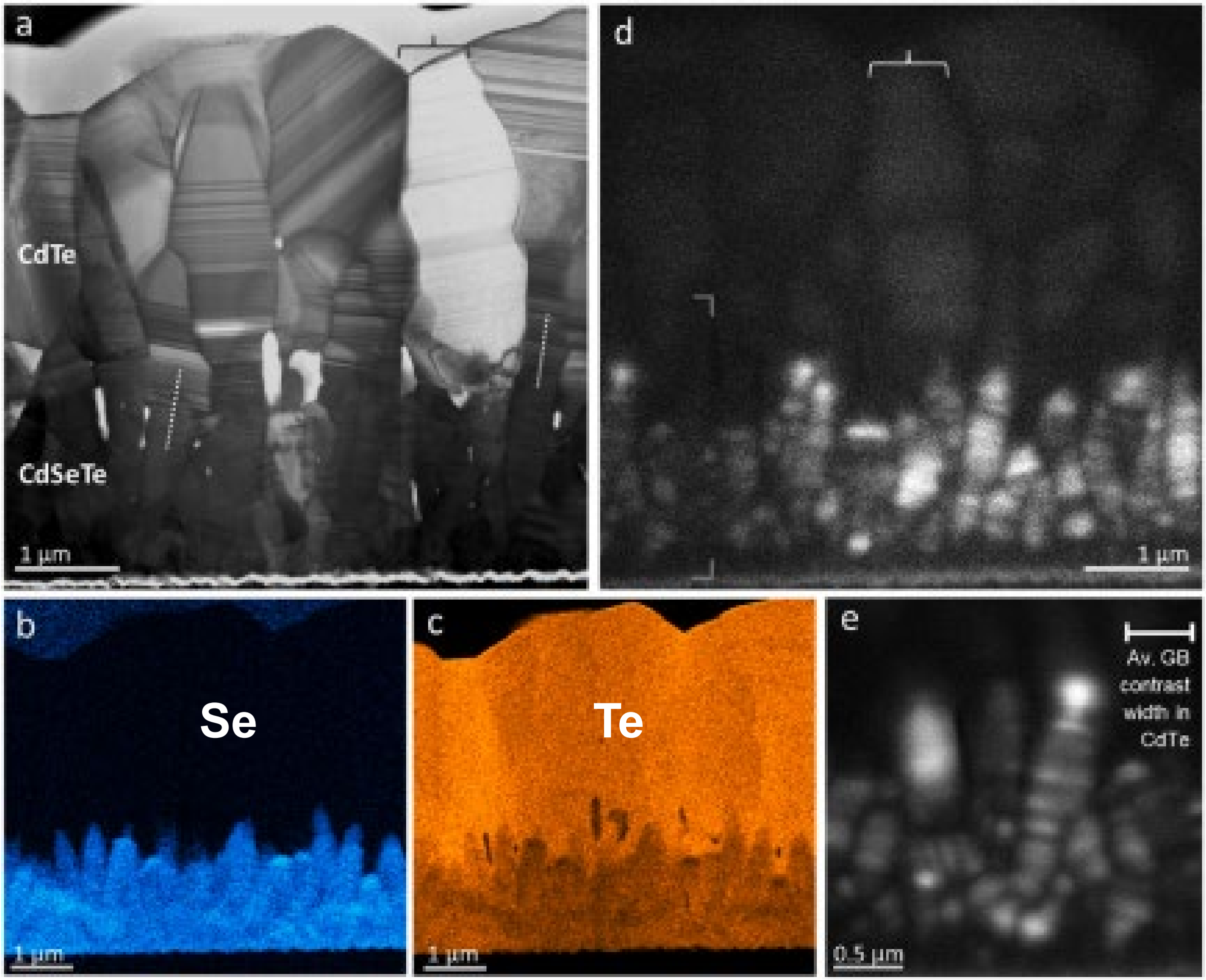
CL TEM Untreated CdSeTe/CdTe device prepared by Xe FIB



Some CL signal seen from CdSeTe without chloride treatment

CdSeTe: Significantly more signal than untreated CdTe

Poor crystalline quality of CdSeTe seen

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Summary

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CdSeTe precursor : Device performance impacted by combo of CdSeTe thickness and chloride treatment

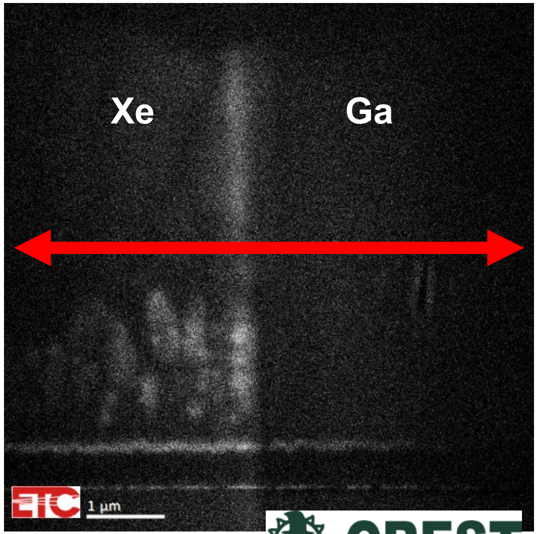
- Thinner is better with moderate $CdCl_2$ (VOC/FF most impacted)
- Insufficient chloride with moderate CdSeTe film, leaves preferred 111 texture and reduced performance

CdSe precursor: Device performance very degraded with residual CdSe

- CdSe Hex/ n-type
- Aggressive chloride needed to form preferred mixed alloy (CdSeTe)

Cl: CdSe (treated) has 50x signal of CdTe

- good device material?
- CdSeTe (untreated) has higher signal than CdTe



Capabilities developed

- Xe-FIB polishing / Large Area EBSD of cross sections

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Acknowledgements

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Colorado State University

Walajabad Sampath
Tushar Shimpi
Jim Sites

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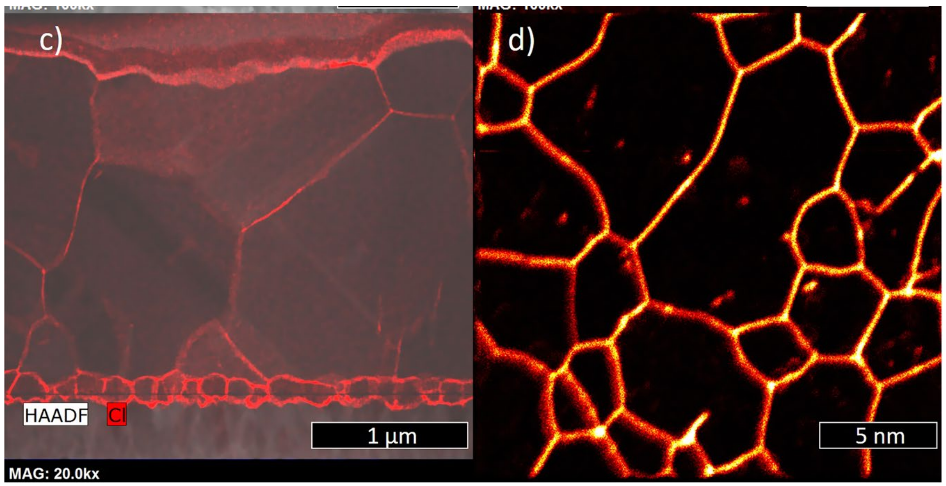
Backup

Role of Chlorine: DFT Results

$CdCl_2$ anneal is critical to high efficiency

- Anneal CdTe in $CdCl_2$, temp > 400 C
- Interdiffusion and grain growth seen



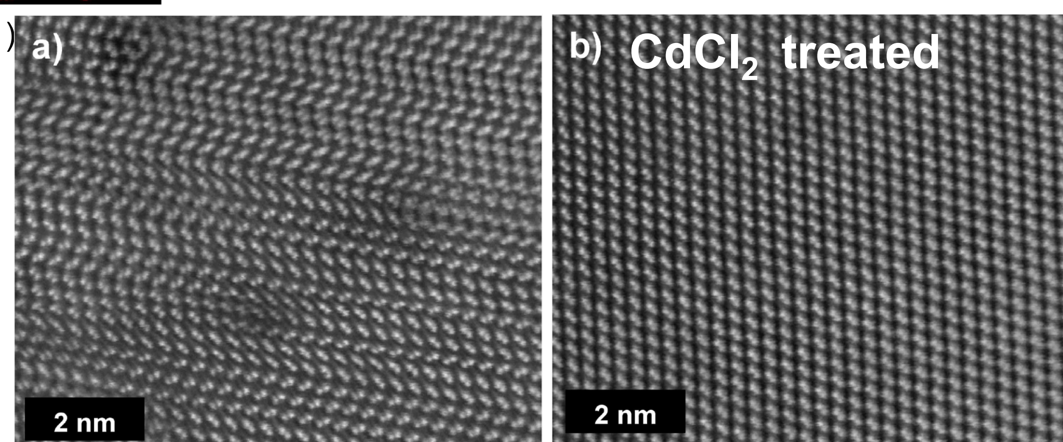
Hatton et. Al. Nature Communications 12, no. 1 (2021)

Analysis:

- TEM/EDS and Cathodoluminescence
- Cl in grain boundaries

Chlorine at grain boundaries drives staking fault removal

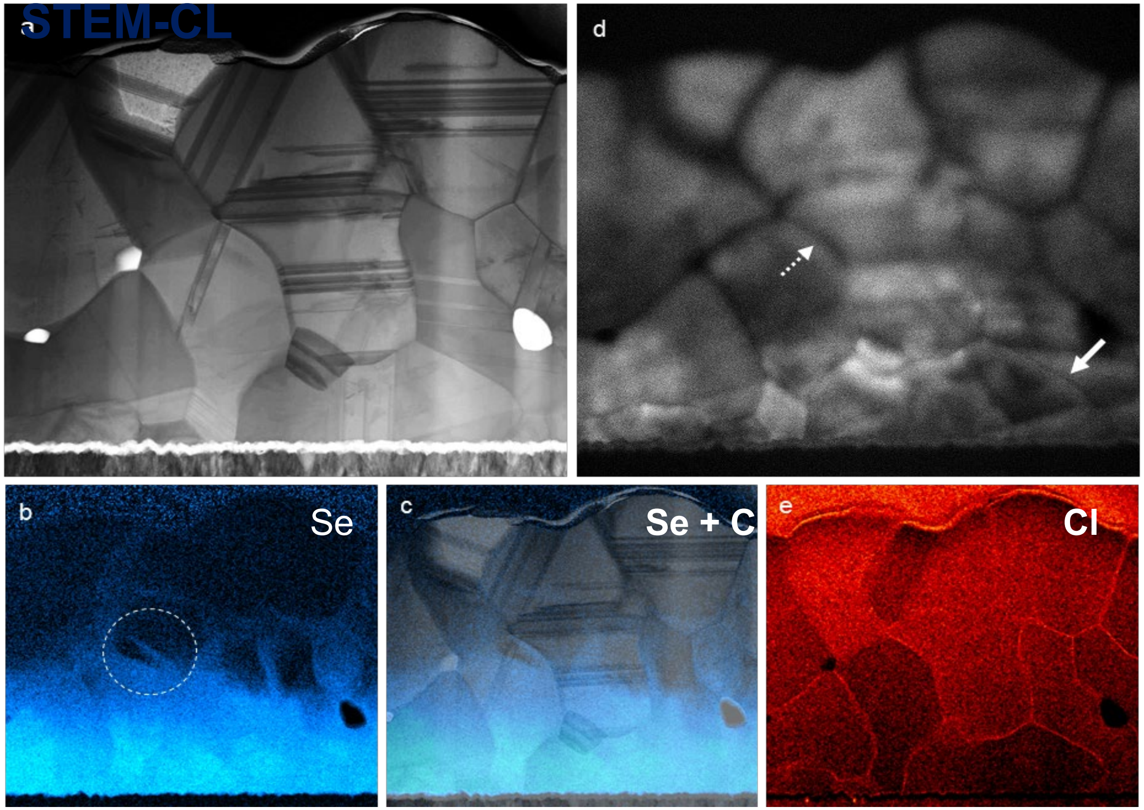
Passivates surfaces



Abbas, A., et. Al. IEEE PVSC 2015

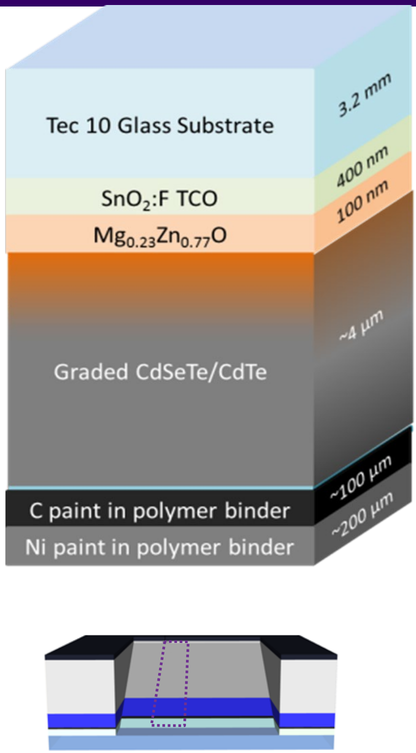
Also See Munshi et. Al. Solar Energy Materials and Solar Cells 186 (2018)

CL with Transmission Electron Microscopy: STEM-CL

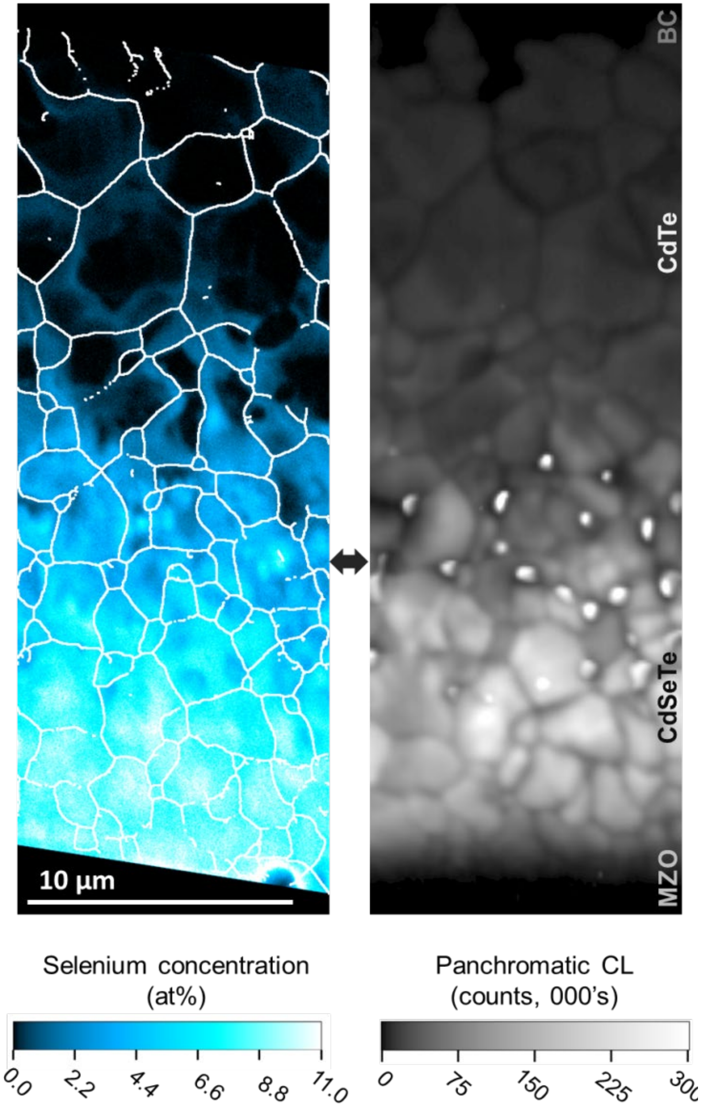


Selenium passivates grain boundaries in alloyed CdTe solar cellsT Fiducia, A Howkins, A Abbas, B Mendis, A Munshi, K Barth, W Sampath,et al...
Solar Energy Materials and Solar Cells 238, 111595 (2022)

Se Passivation



FIB bevel then nano SIMS and CL



Nature Energy 4, no. 6 (2019)

- As-deposited device two distinct films: CdSeTe and CdTe
- Interdiffusion of Se during $CdCl_2$ heat treatment
- Cathodoluminescence (CL) correlation with Se content
- Increased CL signal: Higher quality absorber materials

Se passivates grain interiors

Resulting in higher lifetimes / performance

Interdiffusion of Se into absorber

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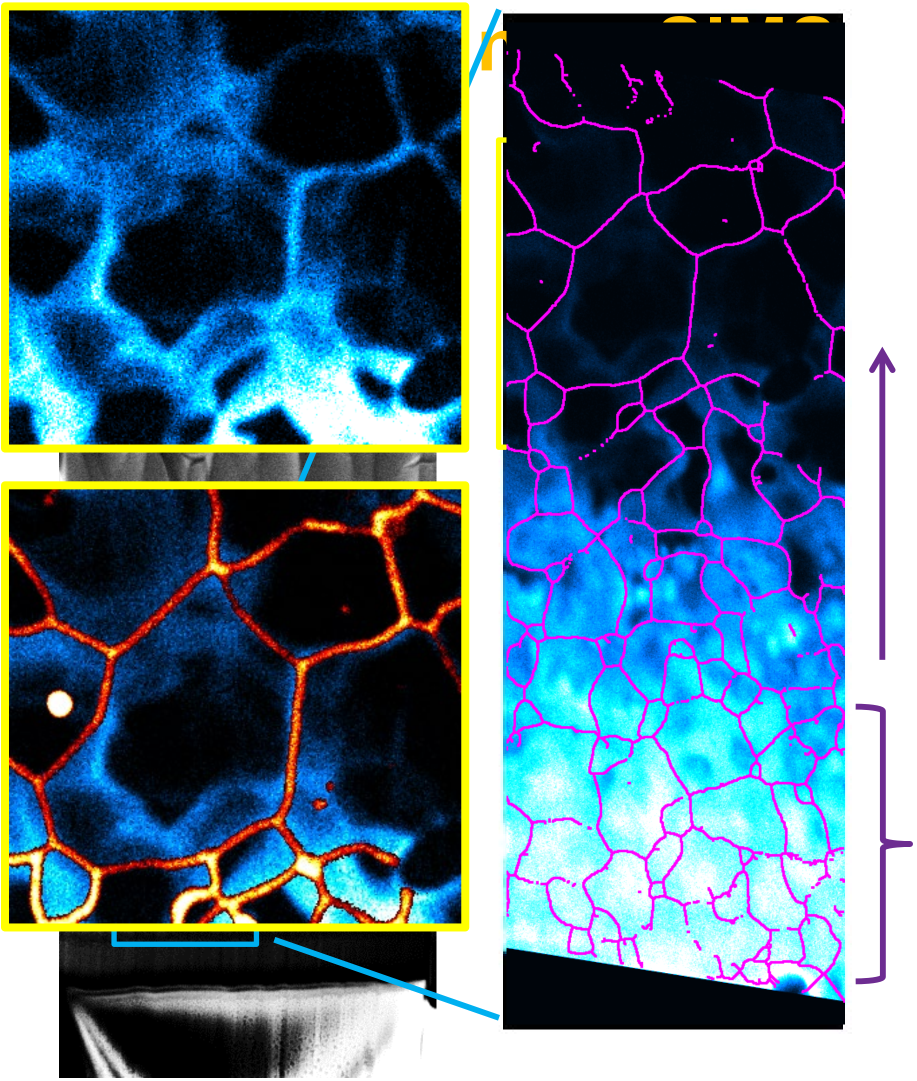

SIMS Se map

- ~10% Se at the front interface
- Interdiffusion into ‘CdTe’ layer above following $CdCl_2$ heat treatment
- Se decoration around grain boundaries
- Diffusion primarily up grain boundaries, then out-diffusion into the bulk

Se passivates grain interiors

Resulting in higher lifetimes / performance

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