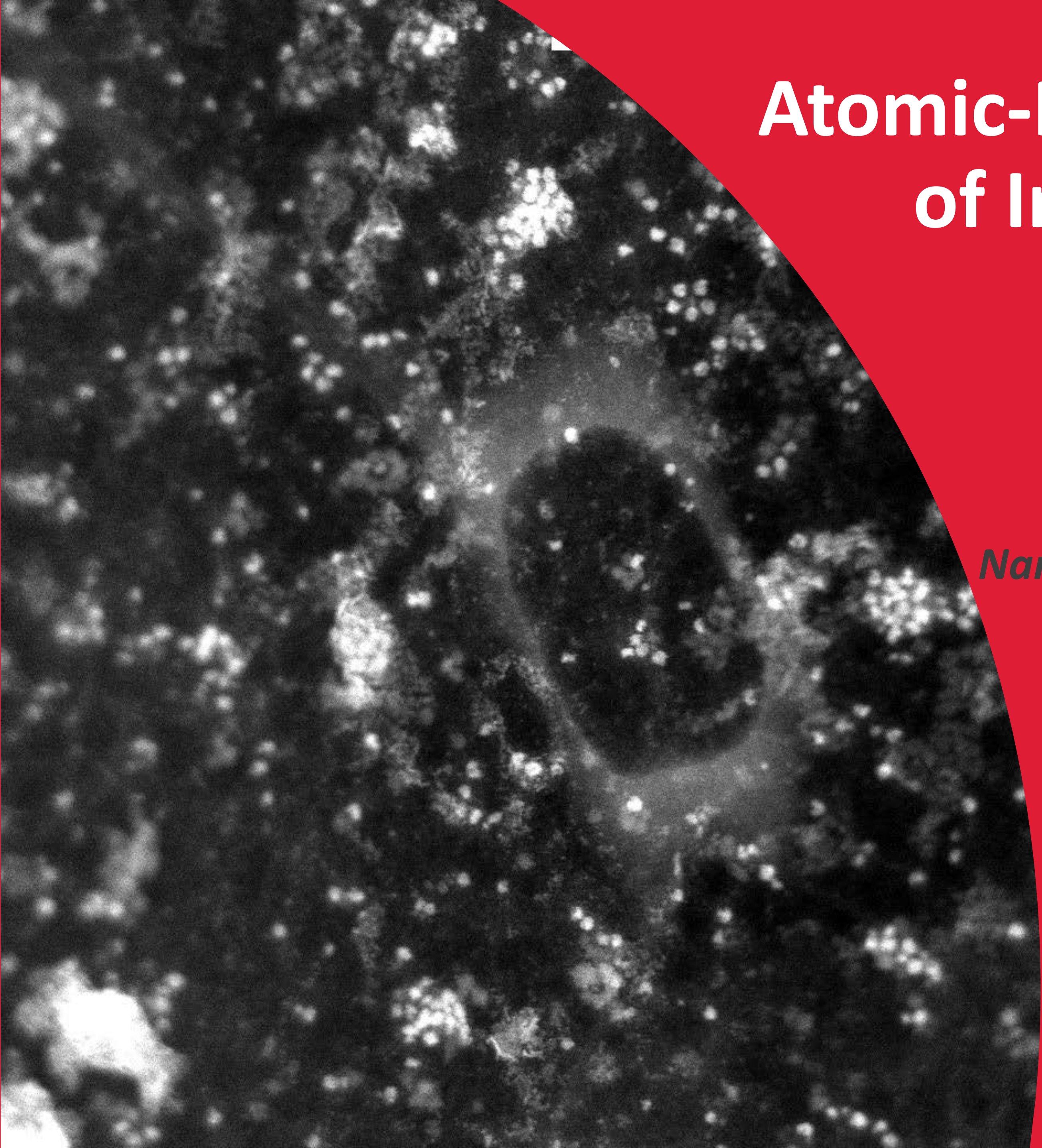

Atomic-Resolution Characterization of Interfaces in Poly-Crystalline CdTe Devices

Robert F. Klie

J. Farrell, J. Guo

Nanoscale Physics Group, Department of Physics

A. Mannodi-Kanakkithodi, M.K.Y. Chan

Argonne National Laboratory

M. Nardone

Bowling Green State University

S. Walajabad and J. Sites

Colorado State University

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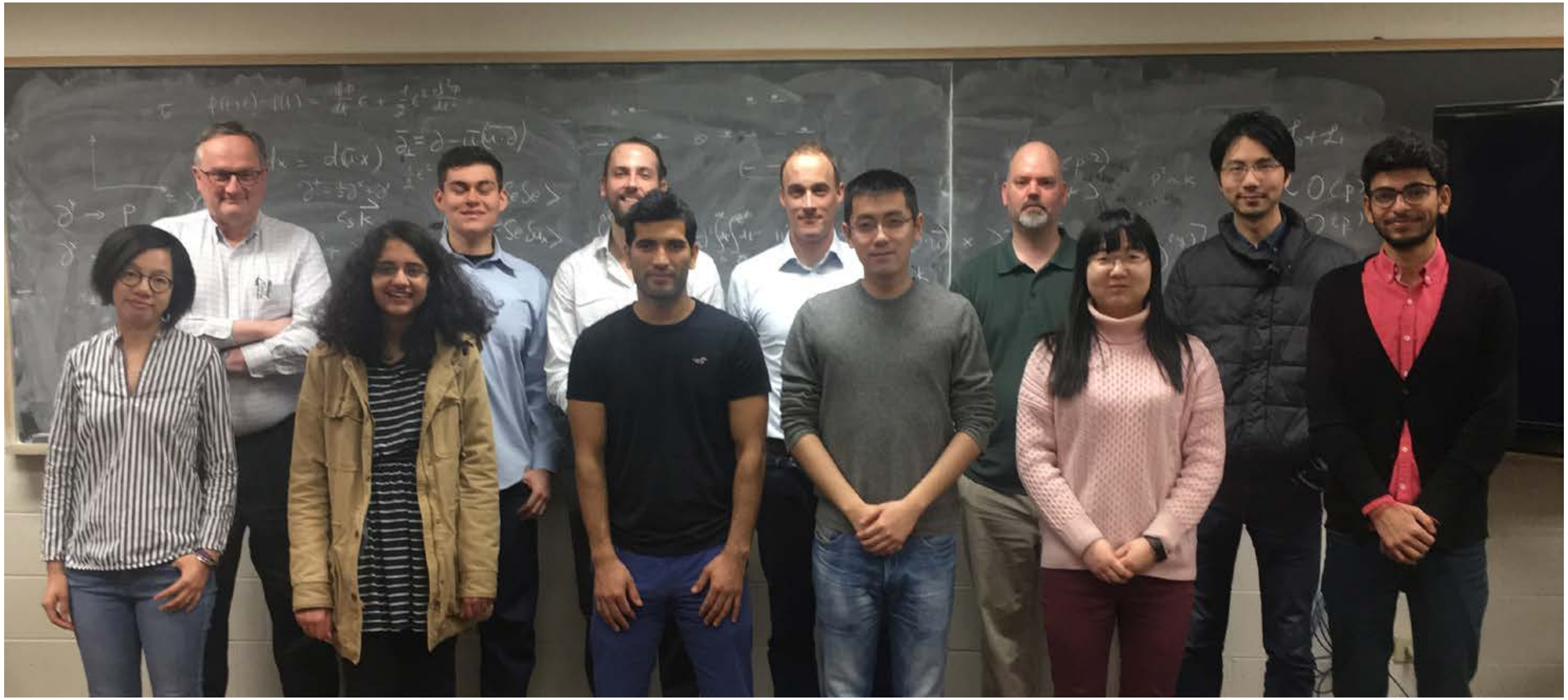

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DOE SunShot EE0007545, EE0008557, EE0008974

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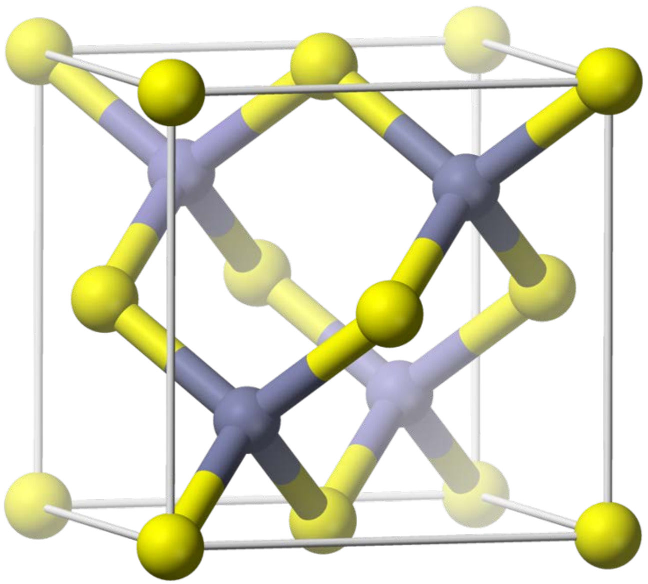
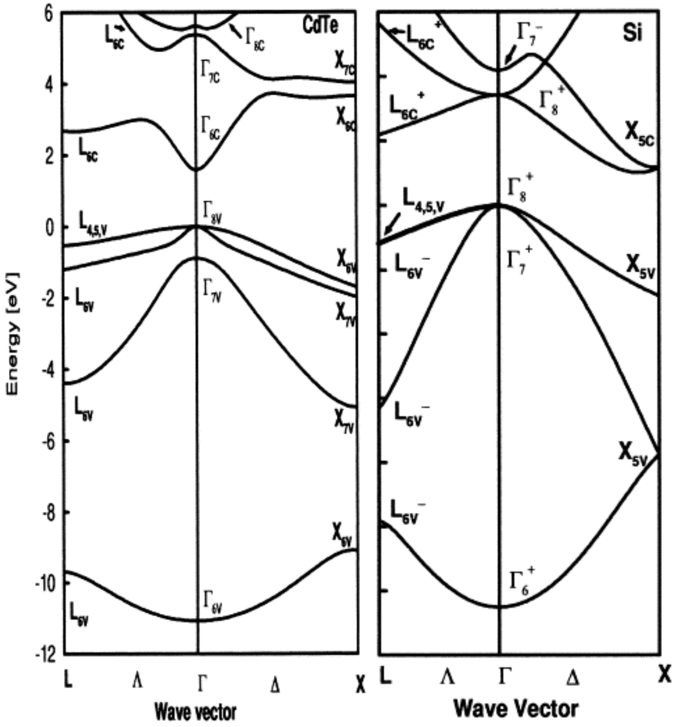
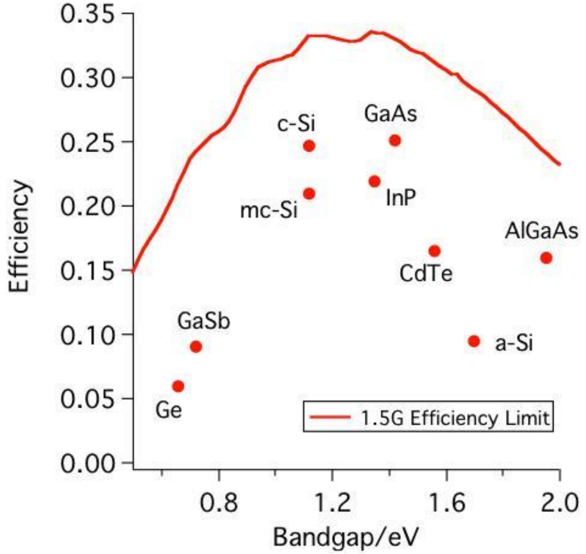
Cadmium Telluride

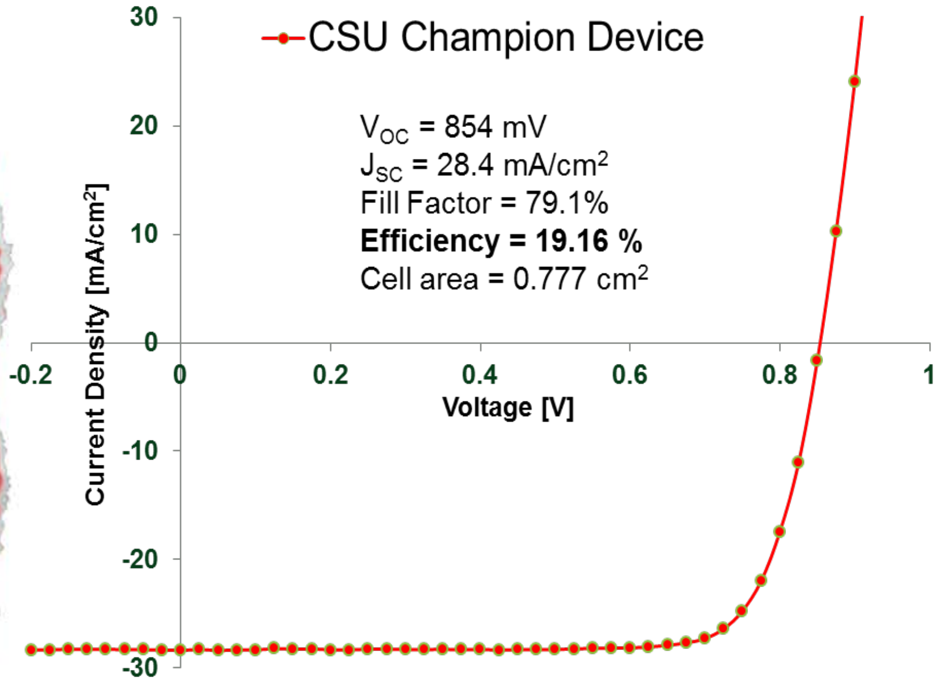




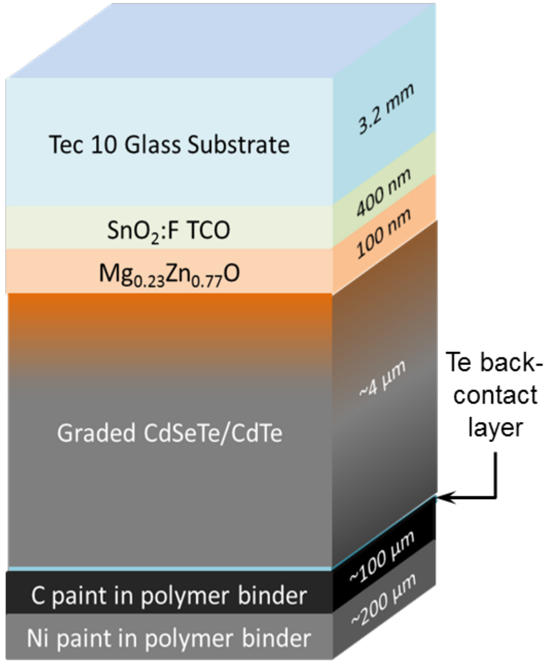


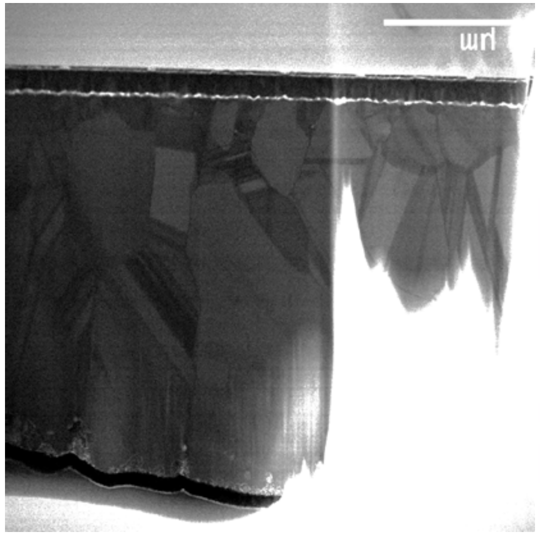
- Nearly ideal direct optical band gap (~1.45 eV)
- High absorption coefficient (99% absorption in 2 µm) enabling thin film technology
- Fast/cheap processing can still yield high efficiency
    - Cost-effective PV devices
    - Economically viable for production

CdTe Solar Cells



No anti-reflection coating





Grain boundaries and interface recombination appear to be the most significant limits!

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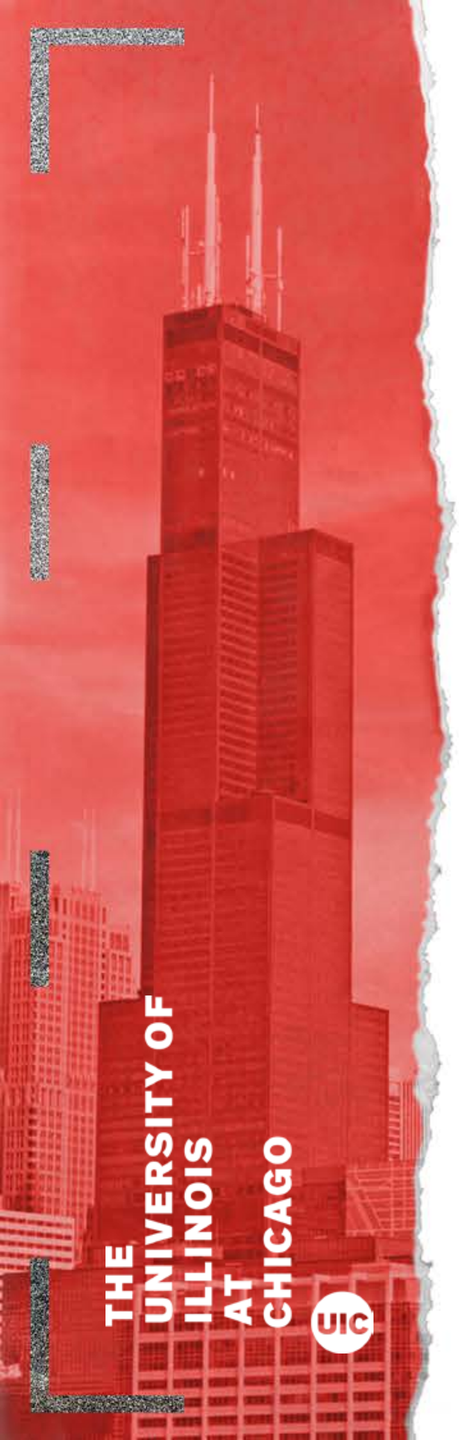
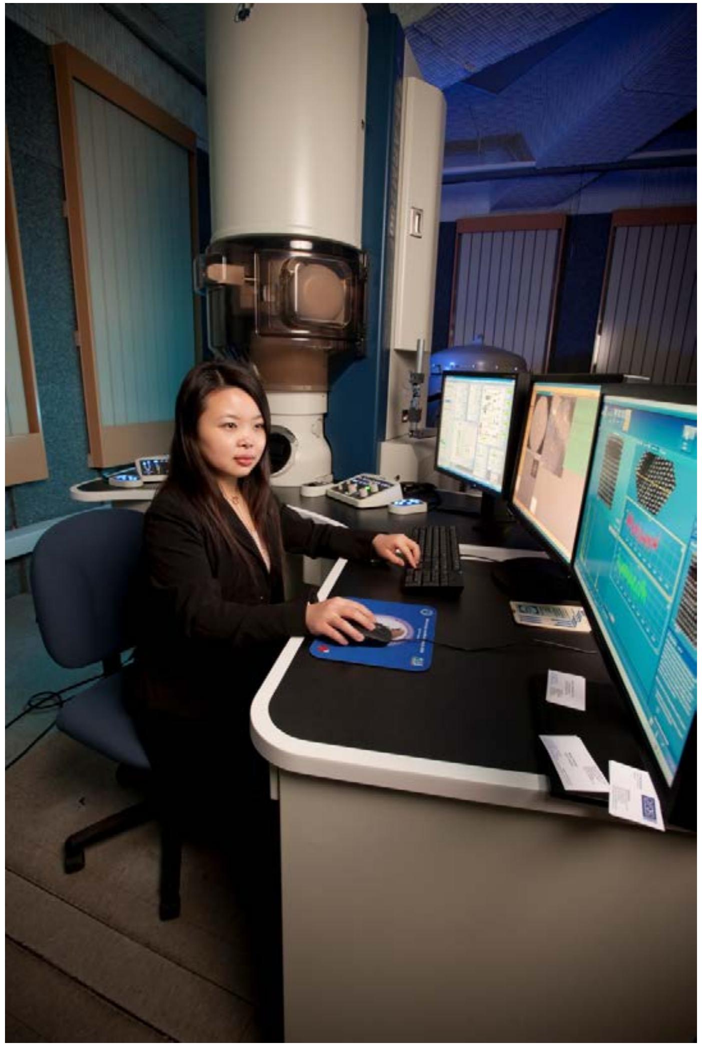


JEOL JEM-ARM 200CF at UIC



- Cold field emission (0.35 eV resolution)
- Probe spherical aberration corrector (less than 70pm spatial resolution)
- Oxford XMax100TLE
- HAADF detectors, BF detector and ABF detector
- Heating, Cooling, Liquid, STM, Vacuum Transfer and Tomography stages.
- Gatan Continuum GIF

NSF – DMR-1408427
NSF – DMR -0959470

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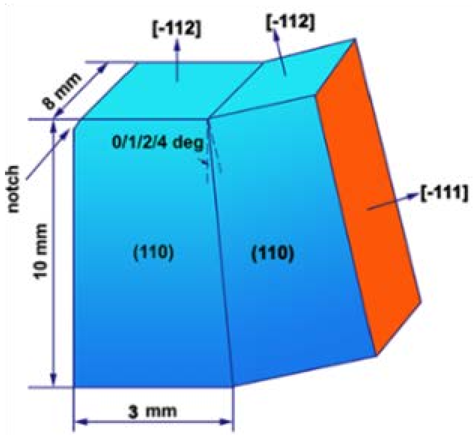
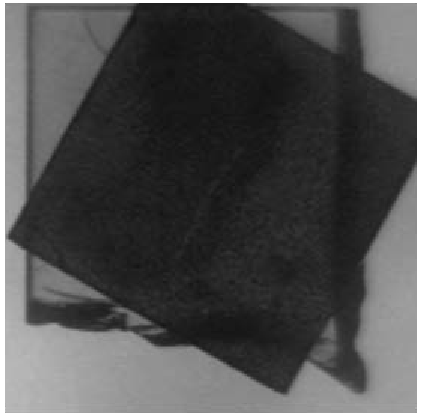
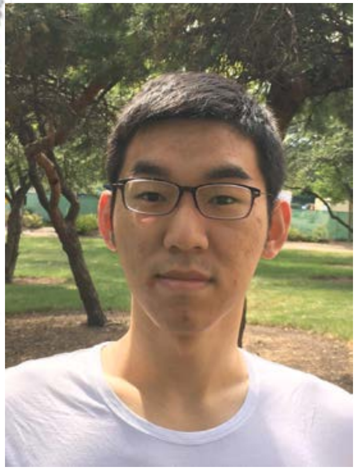
CdTe Bi-Crystals



Schematic of bi-crystal



IR image of bi-crystal



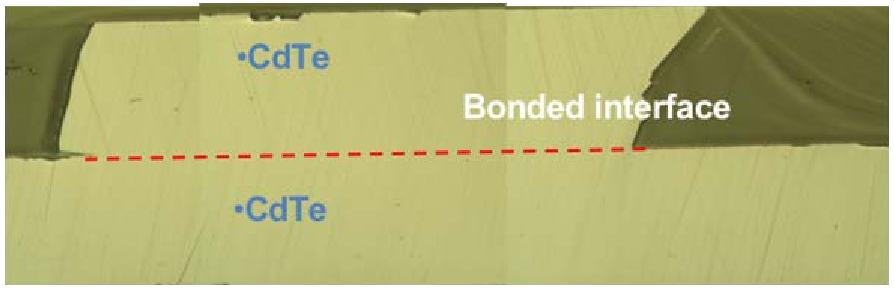


Image of bi-crystal

- CdTe (111) wafers
  - $[112]_1//[011]_2$
  - $[0\text{-}11]_1//[01\text{-}1]_2$
  - $[0\text{-}11]_1//[0\text{-}11]_2$
  - Small angle (5º) Tilt
  - Small angle (2º) Tilt
- CdTe (110) wafers
  - $[1\text{-}1\text{-}2]_1//[\text{-}111]_2$
  - Small angle (4º) Tilt
- CdTe (100) wafers
  - $[011]_1//[011]_2$
- CdTe (211) wafers
  - $[0\text{-}11]_1//[01\text{-}1]_2$
- CdZnTe (111) wafers
  - $[0\text{-}11]_1//[011]_2$
- CdTe (100)/CdTe(110)
  - $[0\text{-}11]_1//[\text{-}111]_2$
- CdS (001)/CdTe (111)

Jinglong Guo

in collaboration with M. Chan (ANL) Moon Kim (UT Dallas), A. Rocket (CSM) ad M. Nardone (BGSU)

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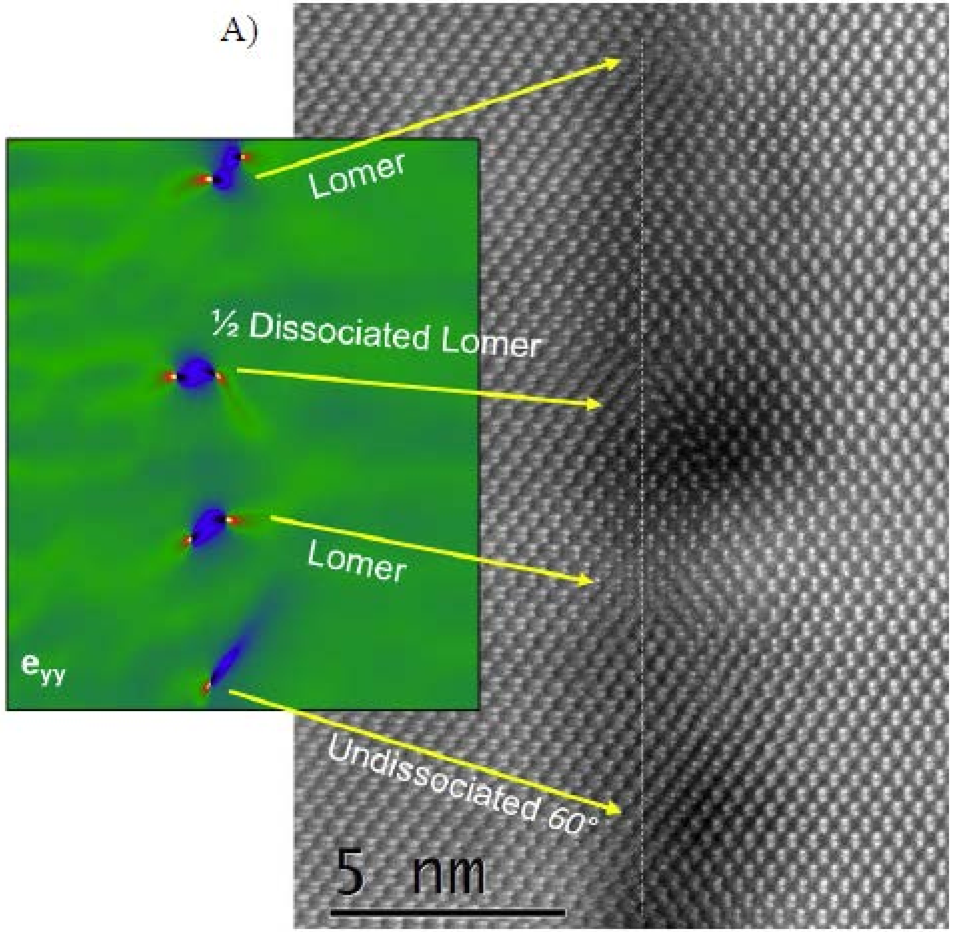
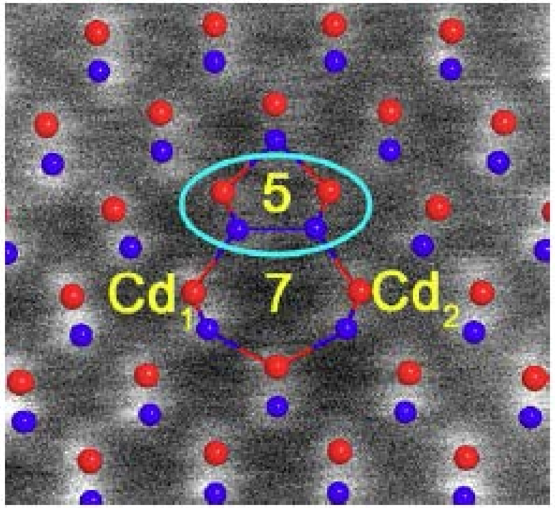
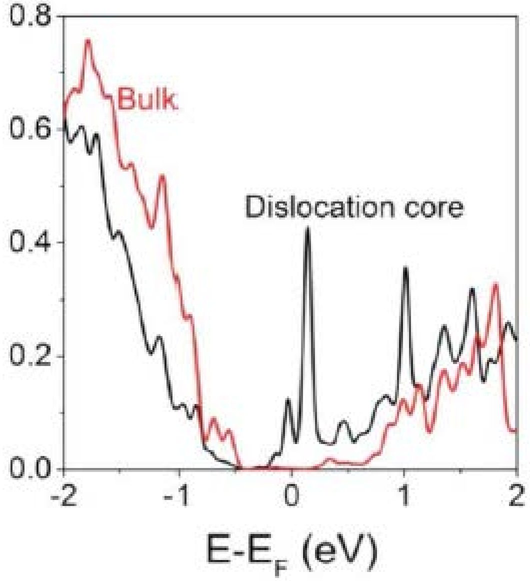
CdTe Bi-Crystals



Paulauskas, PhD Thesis, University of Illinois – Chicago (2016)





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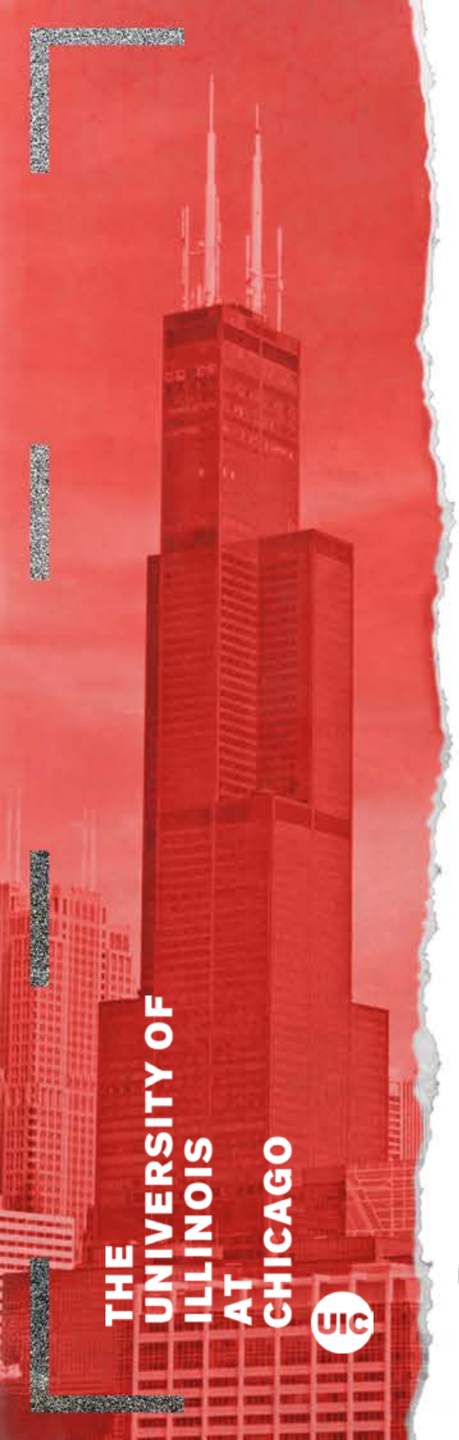
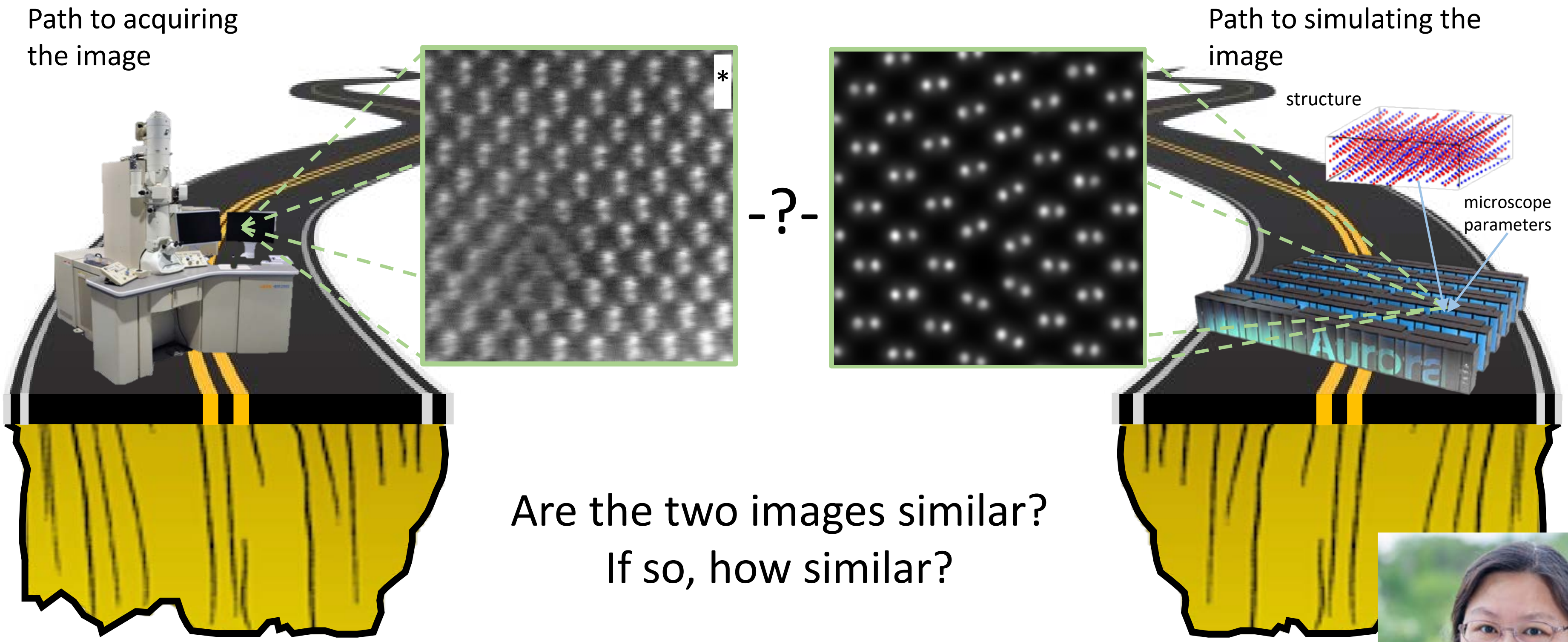


CdTe Grain Boundaries

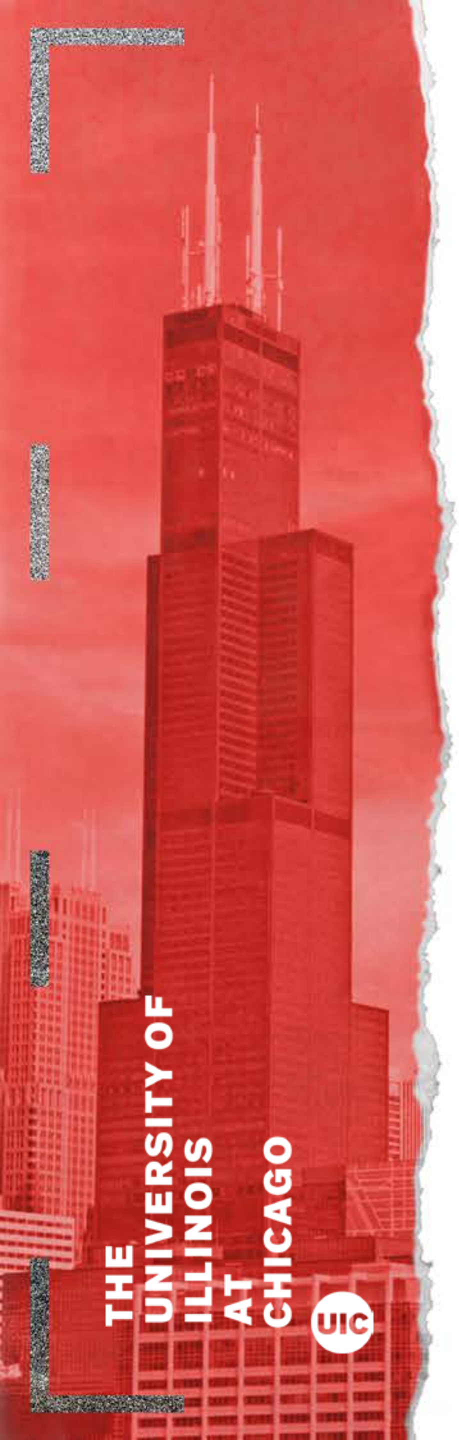
Automate the matching of experimental and computed images



Are the two images similar?
If so, how similar?

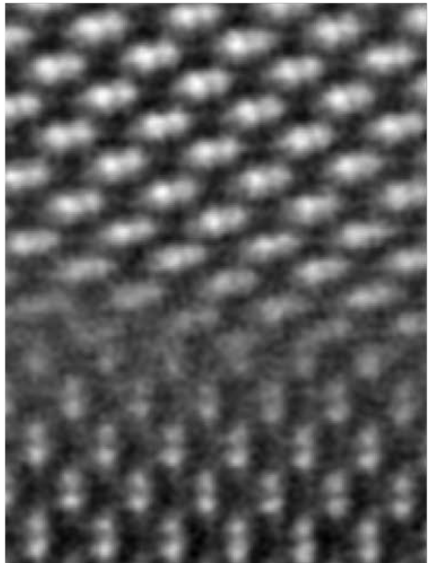
Maria Chan (ANL)

E. Schwenker et al, “Image Matching for Automated Comparisons in Atomic-Resolution Electron Microscopy,” in preparation.

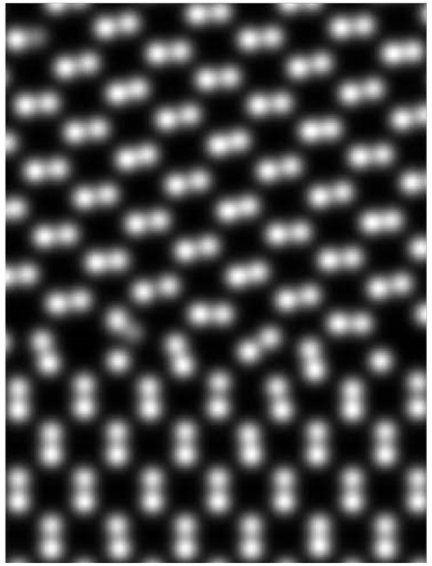


CdTe Modeling

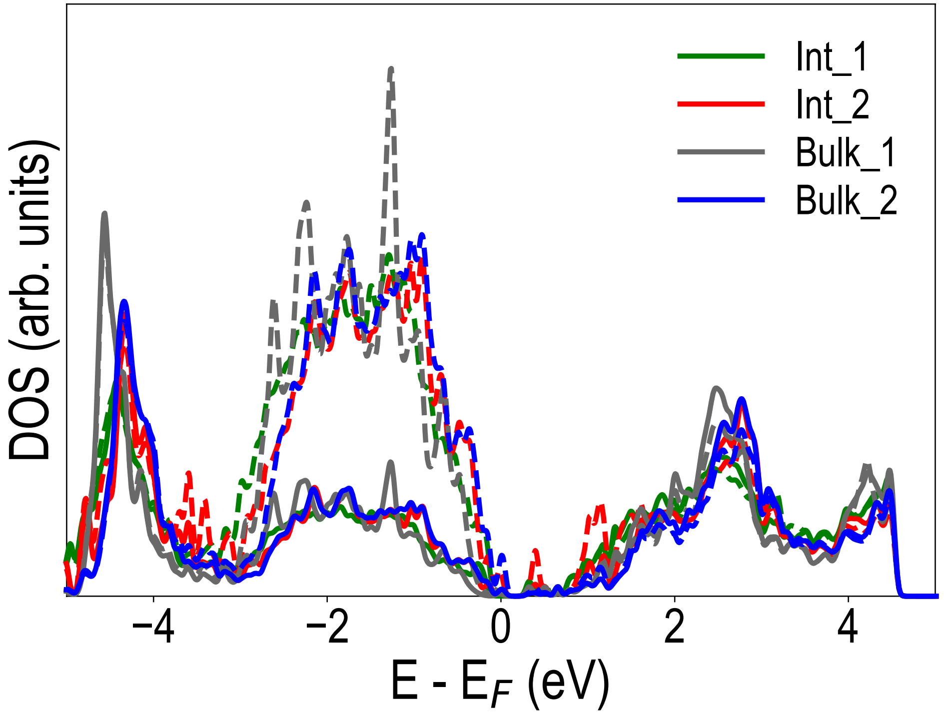
Original STEM GB image



Convolution image simulation



Overlay



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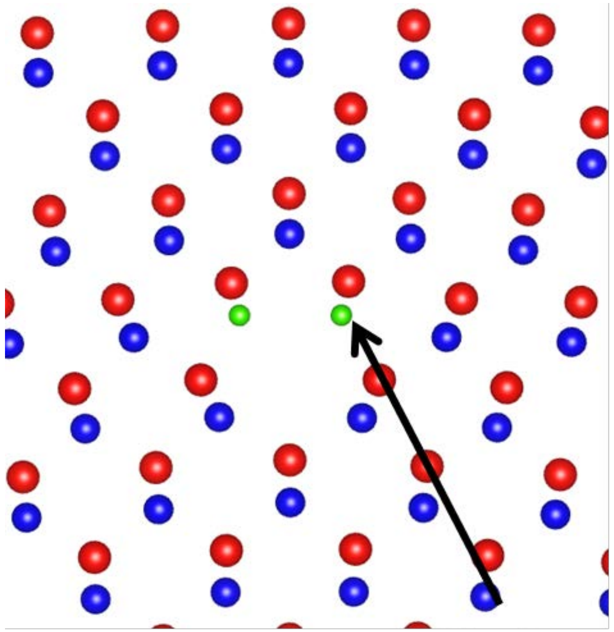
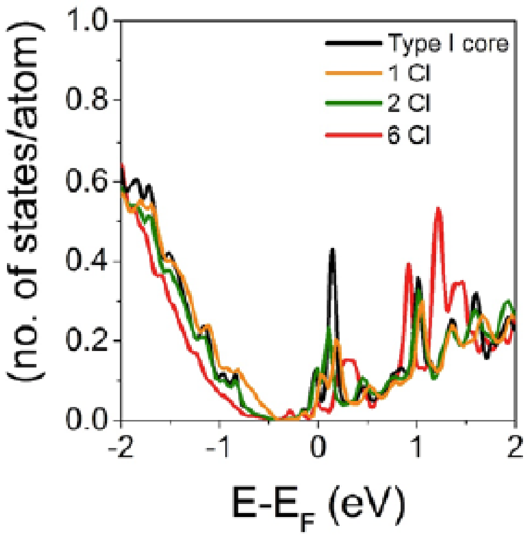
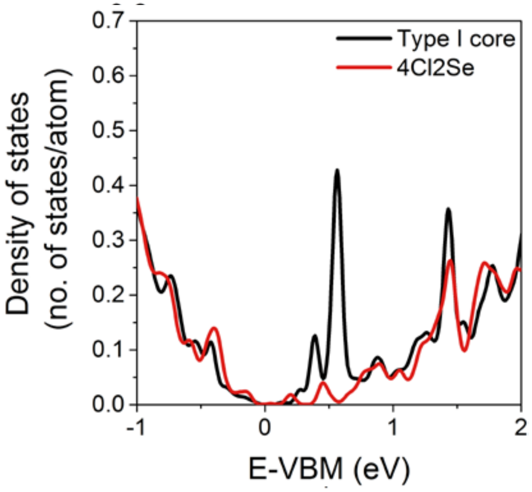
CdTe Modeling



Cl, Se





- Cl , Se can passivate defect states in the mid-gap.
- Cl and Se segregation of dopants to grain boundaries is thermodynamically favorable.
- Co-doping Se+Cl further reduces mid-gap states when substituted to dislocation core.

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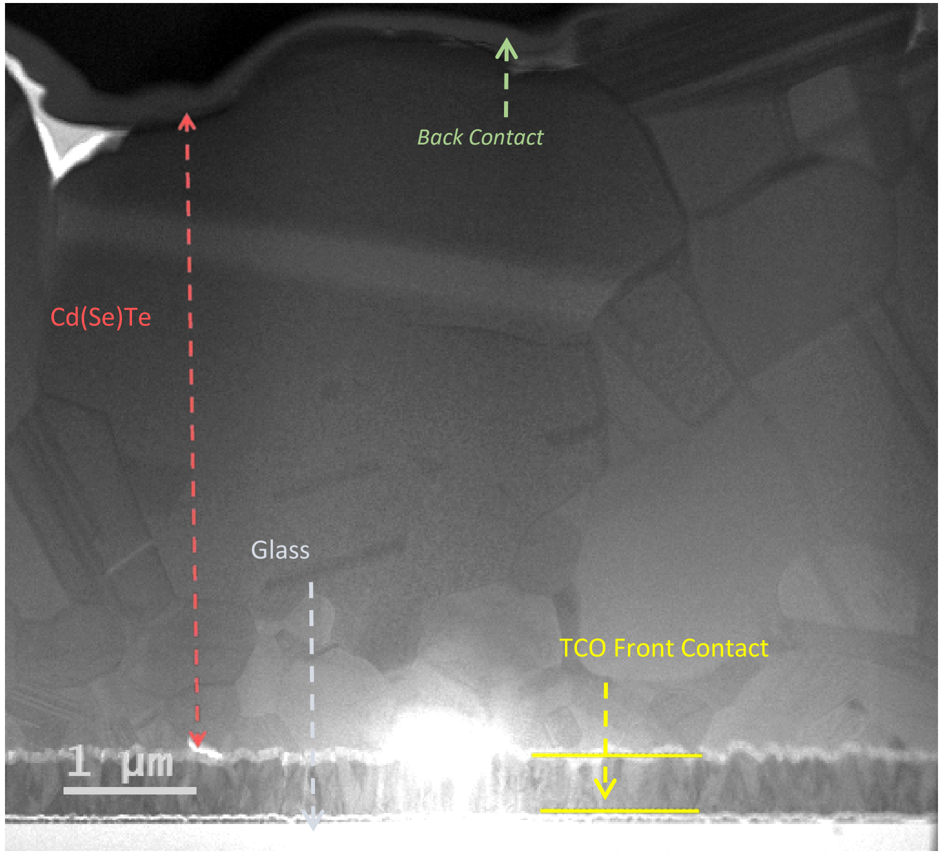
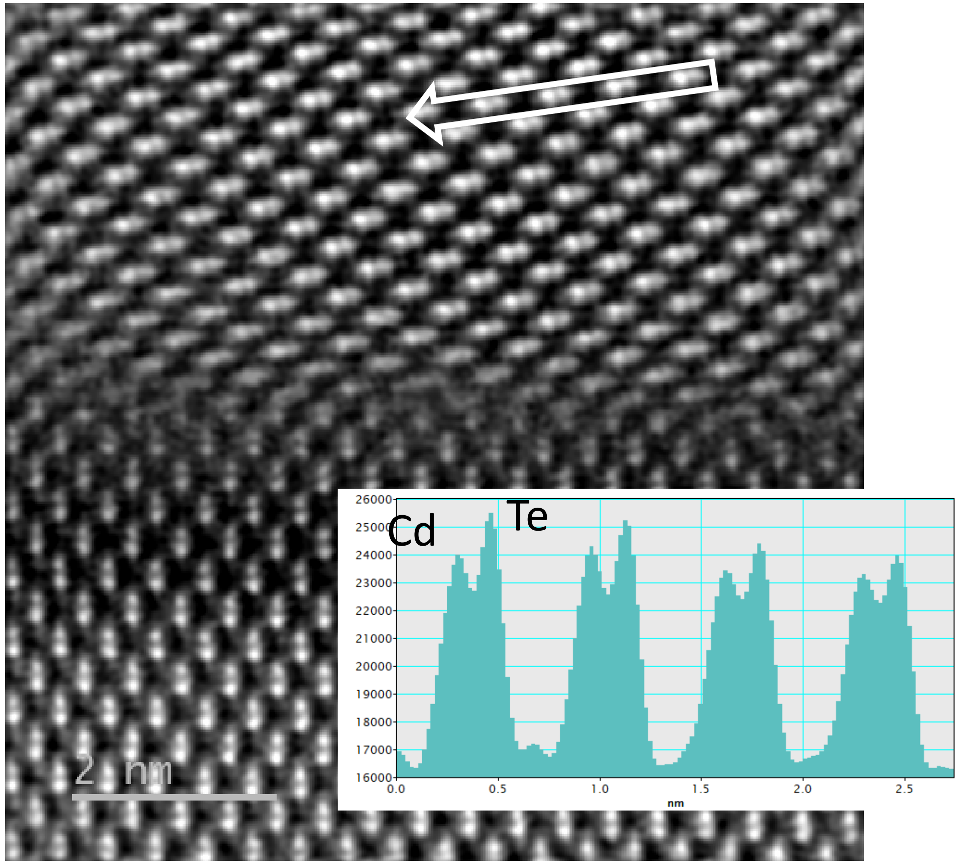
Imaging CdSeTe Devices

Cross-section ABF image of CdTe cell

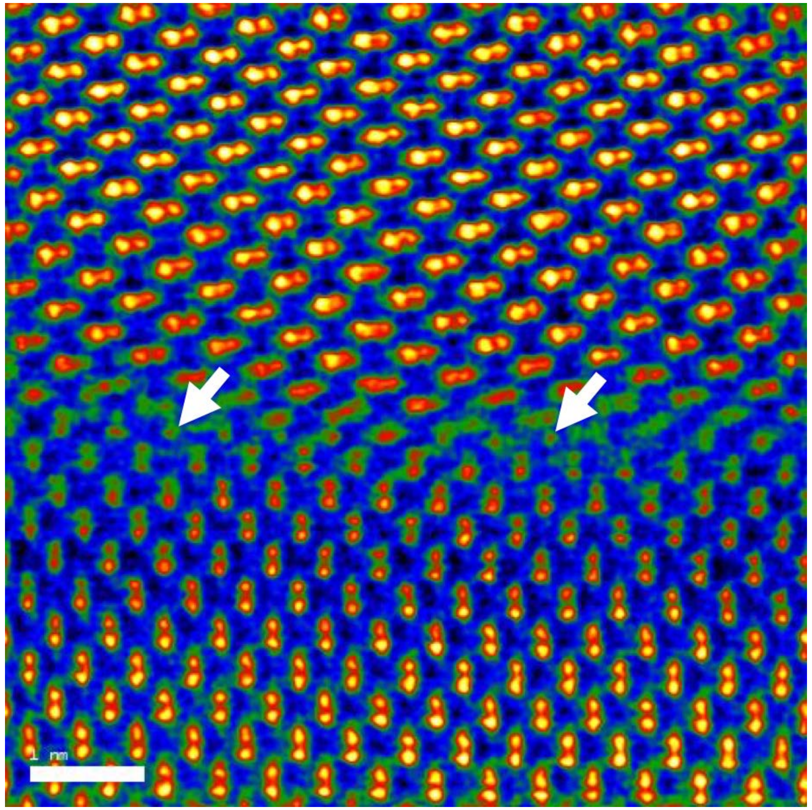


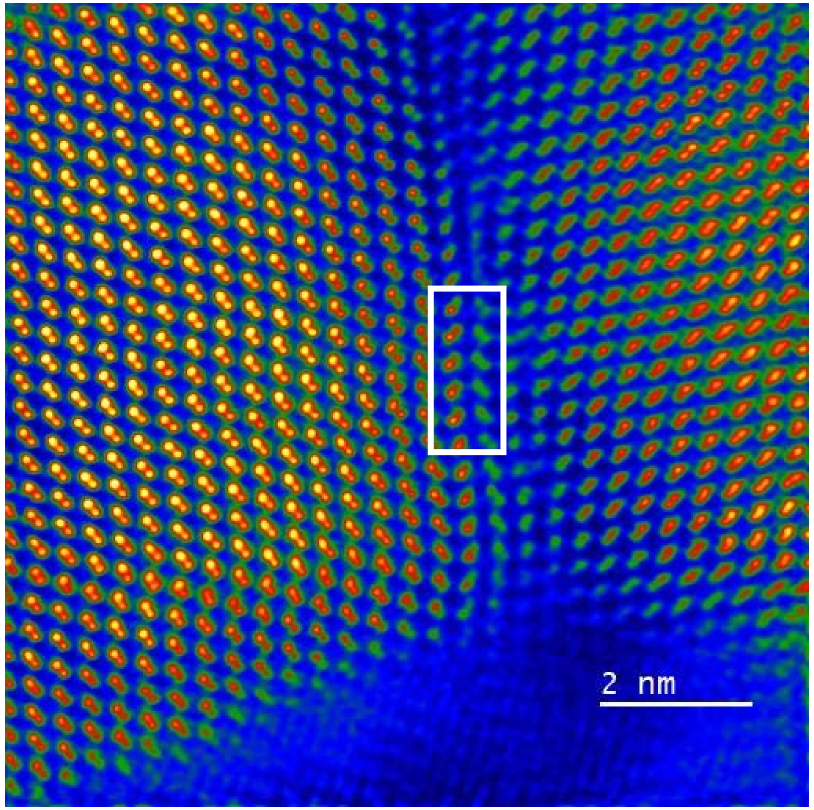
Atomic resolution HAADF image of grain boundaries in CdSeTe solar cell



From atomic-resolution Z-contract imaging, individual columns can be identified.

Imaging CdSeTe Devices





Atomic structure of CdSeTe grain boundaries unaffected by alloying.

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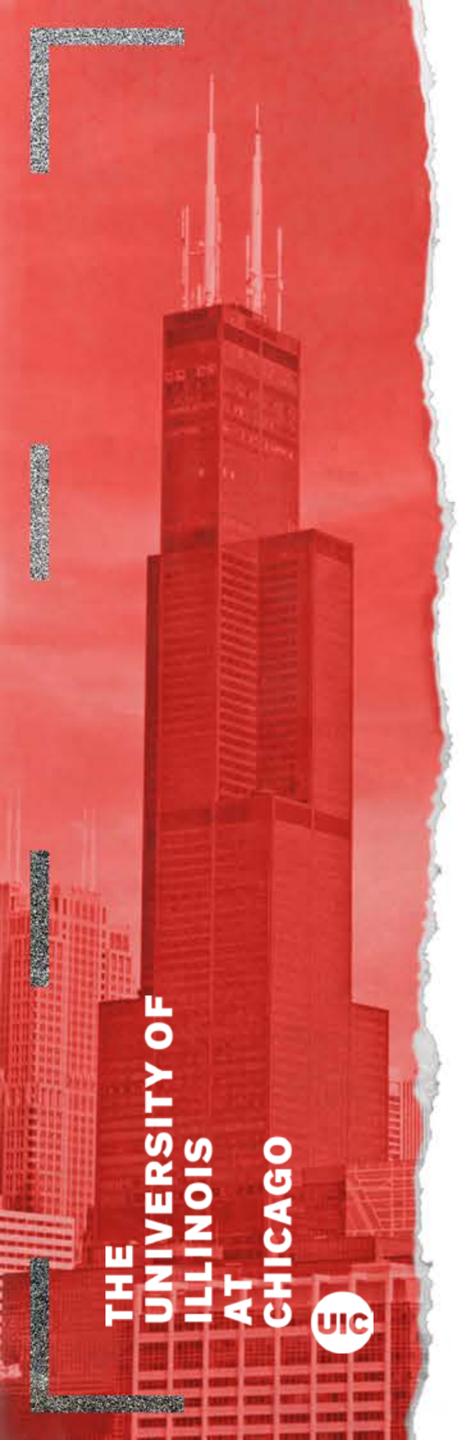
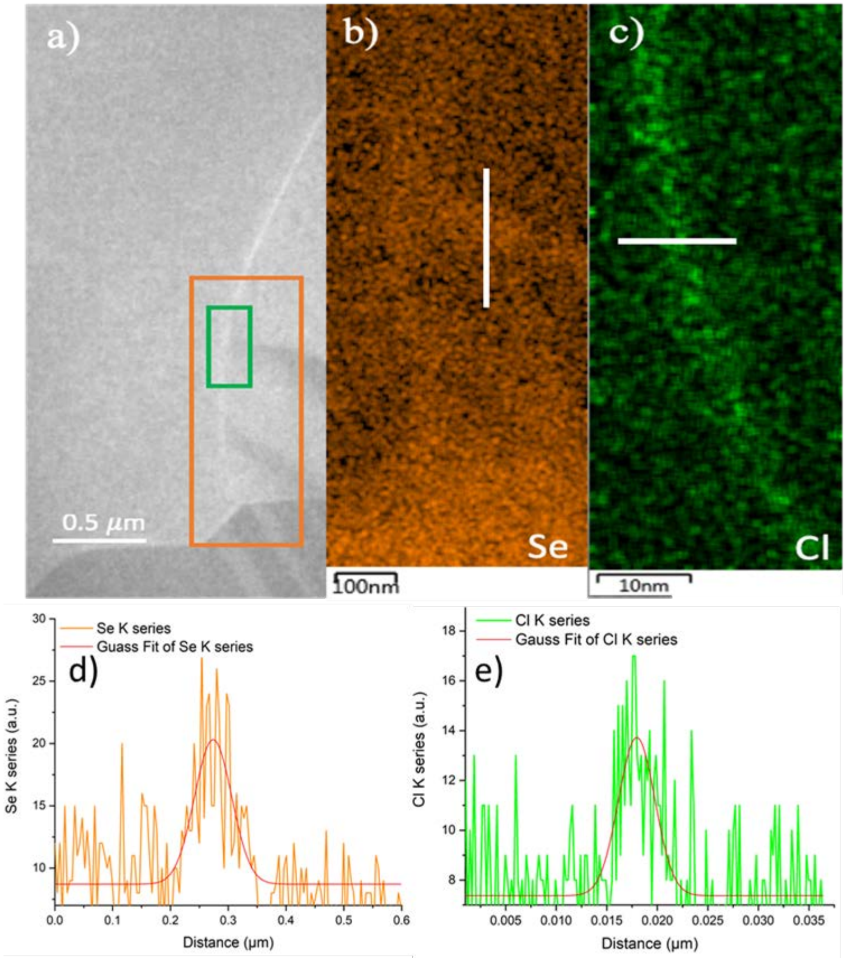
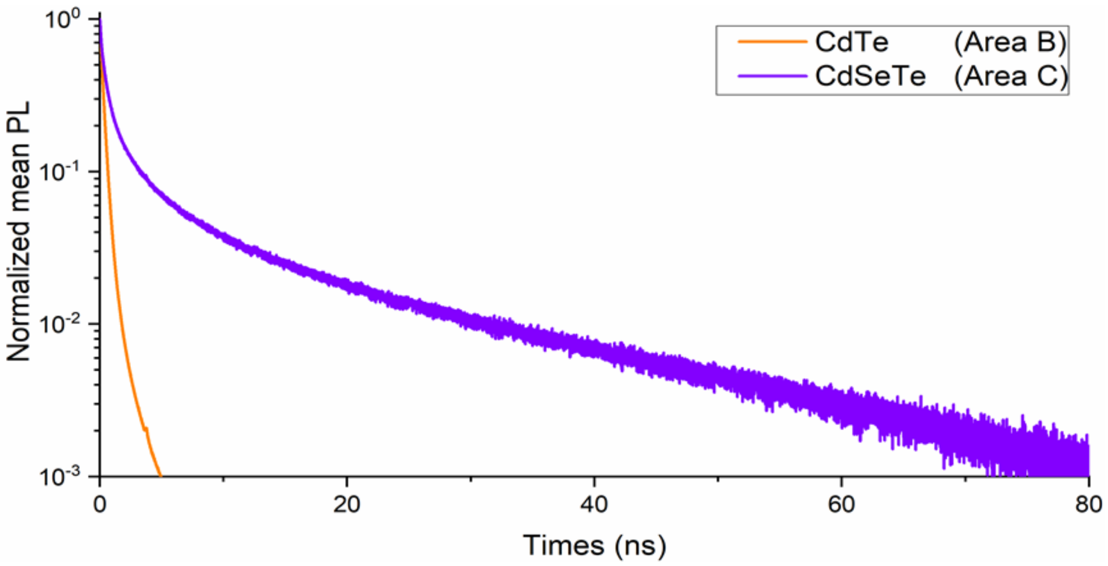


Grain boundary effects





- **Cl and Se co-passivate grain boundaries**
- **Increase in carrier lifetime**

"Effect of selenium and chlorine co-passivation in polycrystalline CdSeTe devices," Guo, J.L., A. Mannodi-Kanakkithodi, F.G. Sen, E. Schwenker, E.S. Barnard, A. Munshi, W. Sampath, M.K.Y. Chan, and R.F. Klie, *Applied Physics Letters*, **115(15),** (2019)

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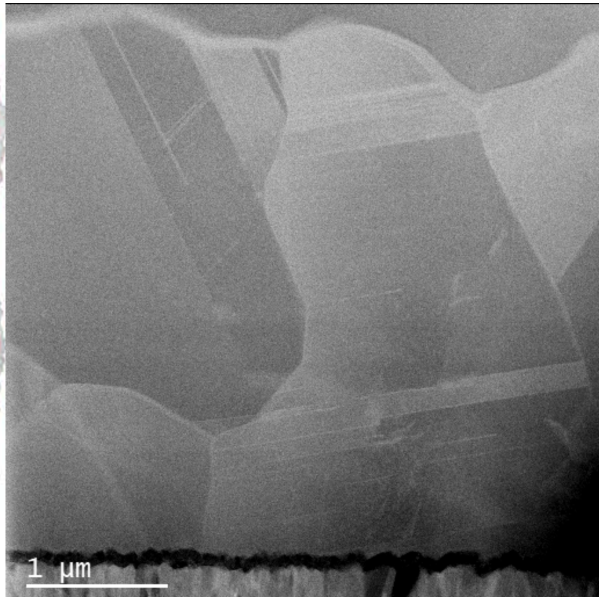
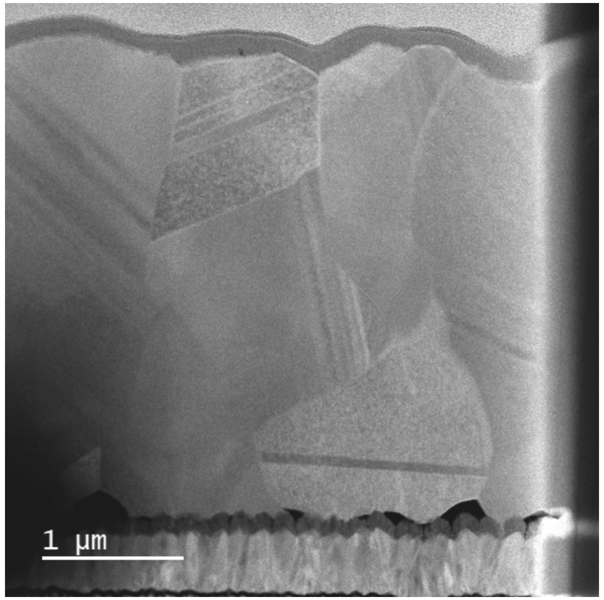
Group V doping in CdTe

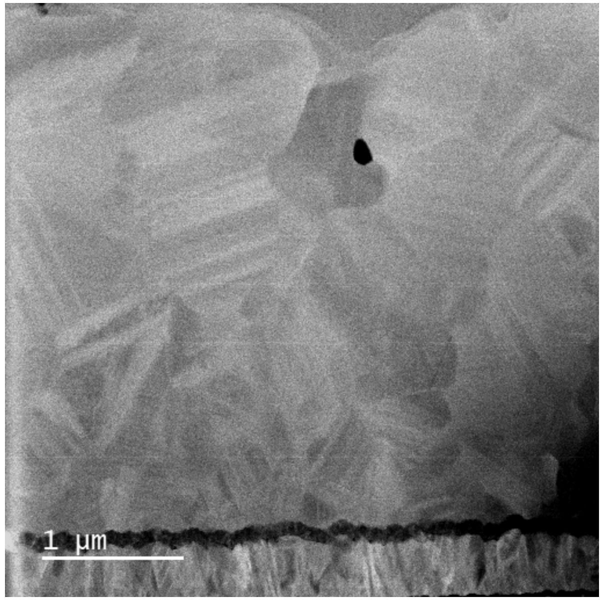
Baseline CdTe (no As)



As-doped CdTe (10^{18} cm^{-3})
Efficiency : 17%~20%



As-doped CdTe (10^{20} cm^{-3})
Efficiency : less than 2%



- Increasing of As doping results in smaller grain size.
- More grain boundaries and dislocations cores.
- More Σ3 boundaries, and more dislocation cores.

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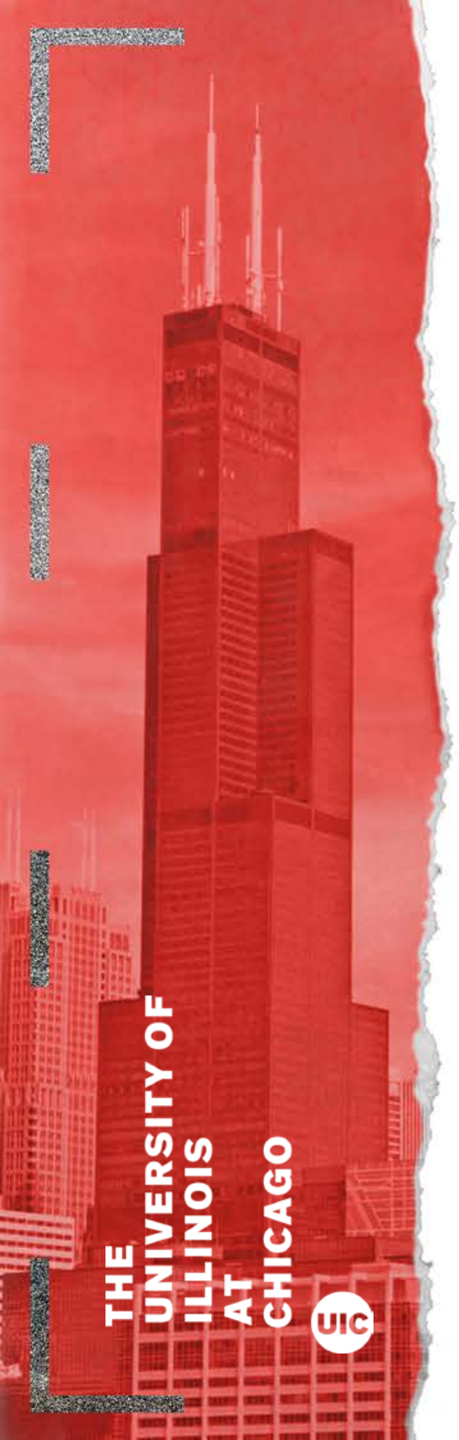
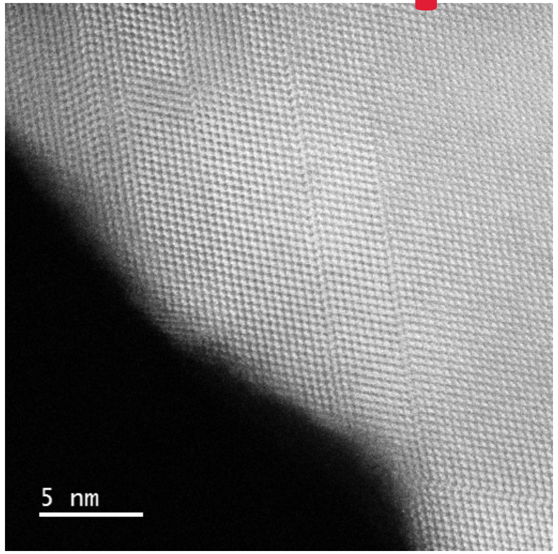
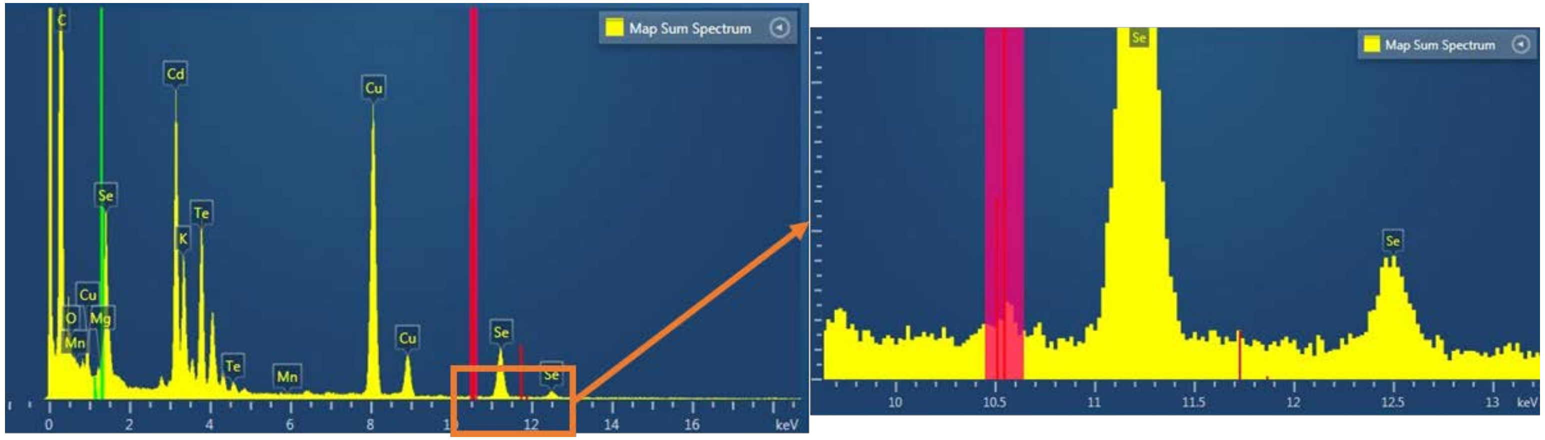


Group V Doping in CdSeTe



- XEDS shows small As signal indicating uniform As distribution in CdSeTe.
- No As-clusters are found.



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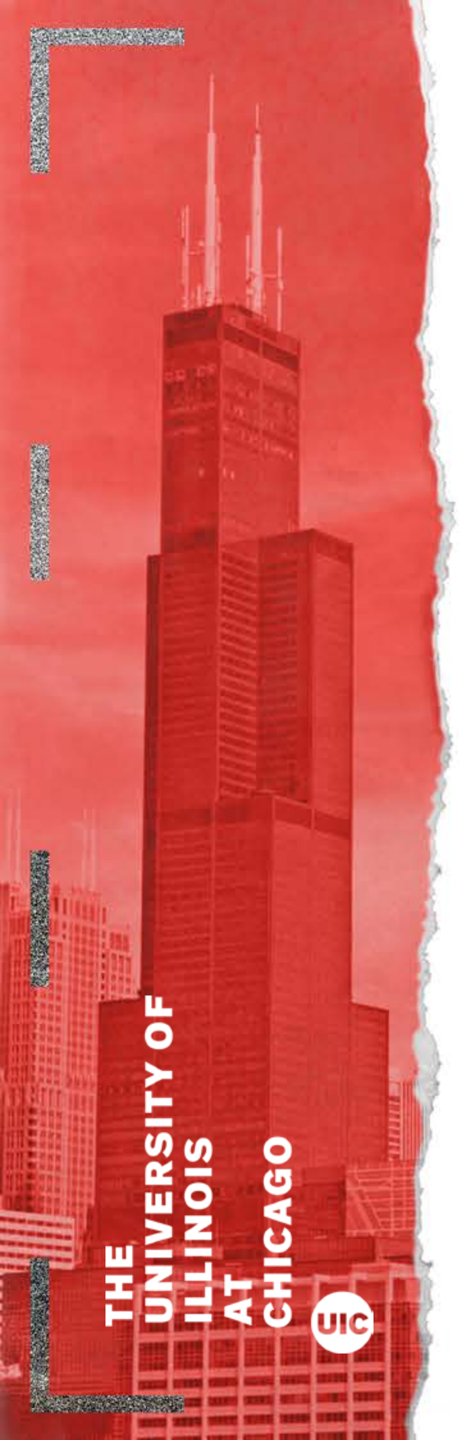

Conclusions

- Model systems are used to determine grain boundary structures.
- Co-passivation for Se and Cl is found to be effective in increasing lifetimes in CdTe devices.
- Group V doping was demonstrated in CdSeTe devices.
- Grain morphology is affected in Group-V doped CdTe devices.

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Questions?