Luminescence Studies on Cu and O Defects in Crystalline and Thin-film CdTe

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Publications:

- "CdTe photoluminescence: comparison of solar-cell material with surface-modified single crystals," App. Phys. Lett., expected publication: May 30, 2005.
- "Photoluminescence Studies on Cu and O Defects in Crystalline and Thin-film CdTe," Proc. Mat. Res. Soc., March 2005.

Outline

- Sample Preparation
- Single Crystal PL Studies
- Thin-film PL Studies
- Theory
- CL Mapping on Thin-film samples
- Conclusions

Sample Used

Single-crystal CdTe:

- p-type, 3 – 5x10^{14} cm^{-3}
- Mechanical polish only
- All Anneals performed at 400ºC for 1hr
- PL taken on treated crystal surface

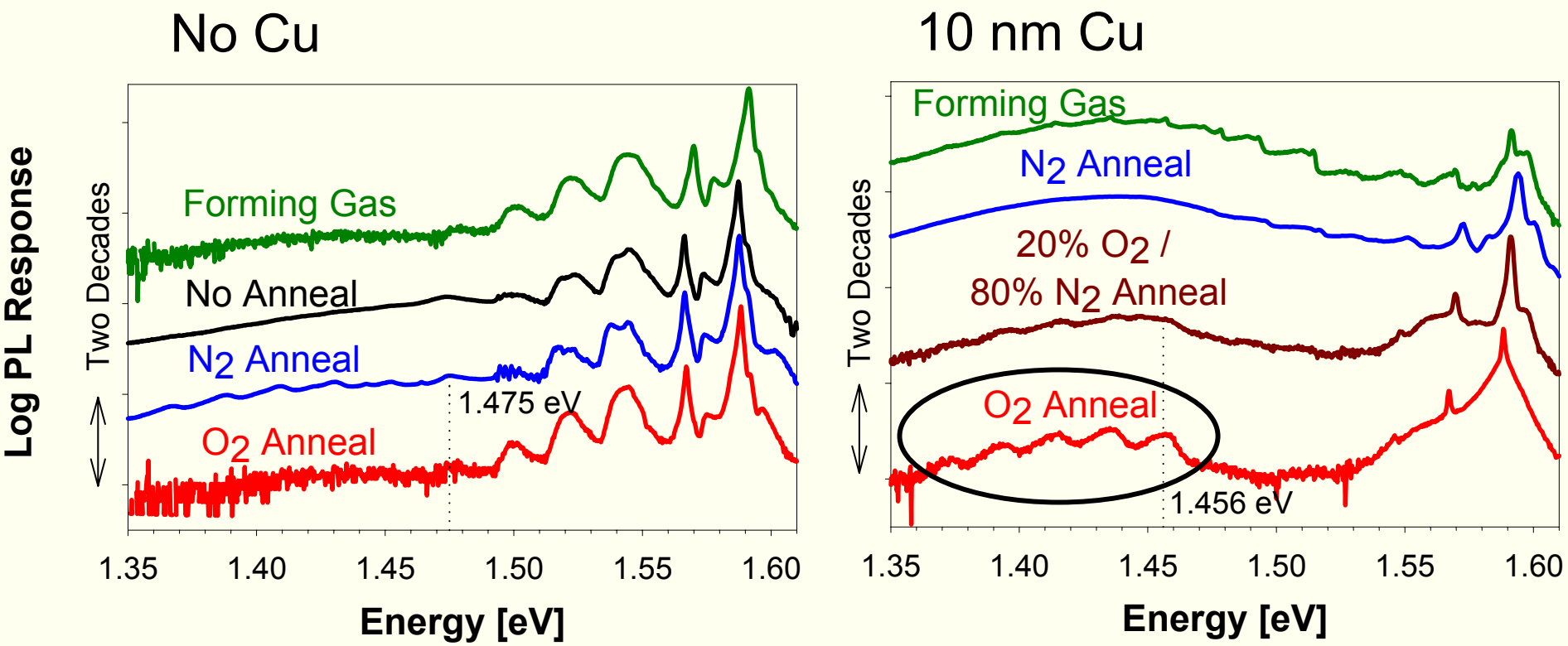
Cu	Anneal Ambient
None	10% H_2 / 90% N_2
	N_2
	O_2
10 nm	10% H_2 / 90% N_2
	N_2
	20% O_2 / 80% N_2
	O_2

Thin-film CdTe:

- Glass/SnO_2:F/CdS/CdTe
- Growth processes:
  - Close-spaced sublimation (CSS)
  - Vapor transport deposition (VTD)
- PL taken on film surface

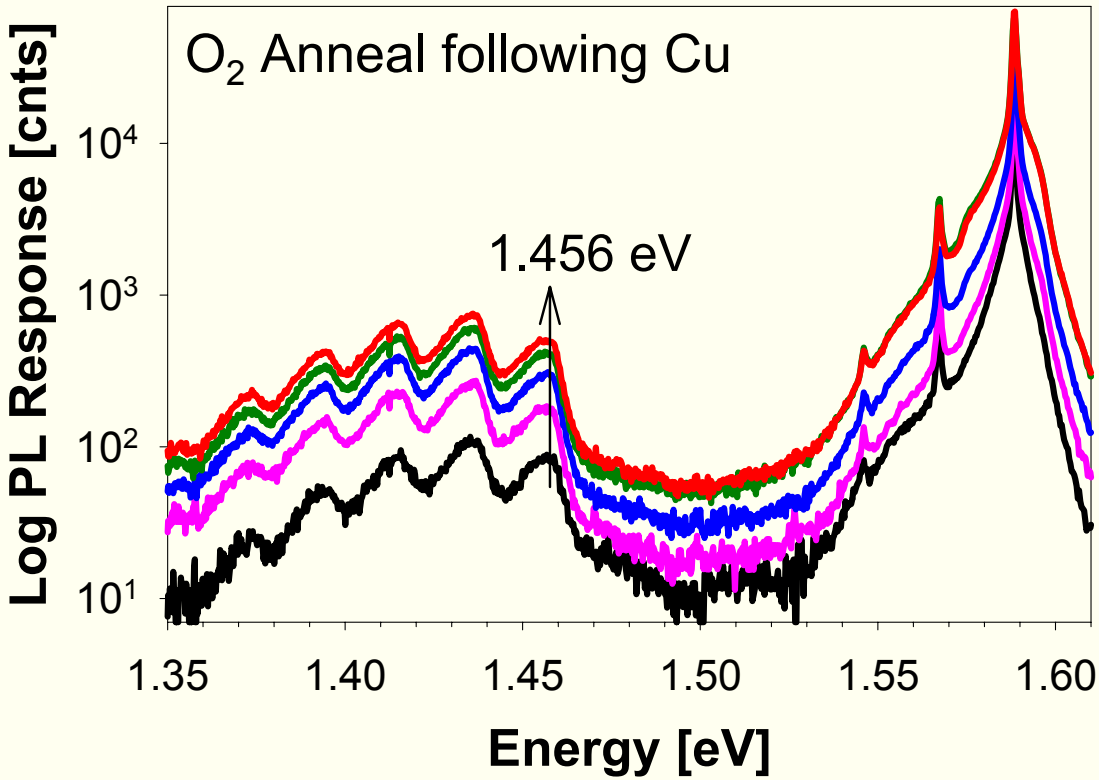
Growth Method	$CdCl_2$
CSS (CSU)	No
CSS (NREL)	No
VTD	No
VTD	Wet

Single-Crystal CdTe

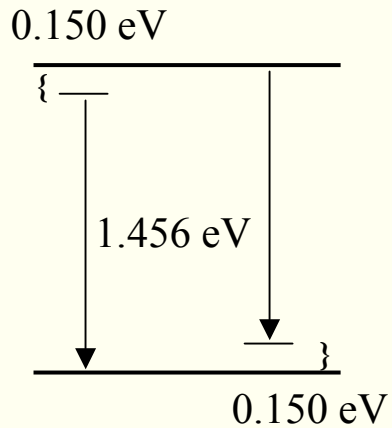


- Only O_2- and air-annealed Cu samples have peak at 1.456 eV

Intensity-dependent PL: Single-Crystal CdTe

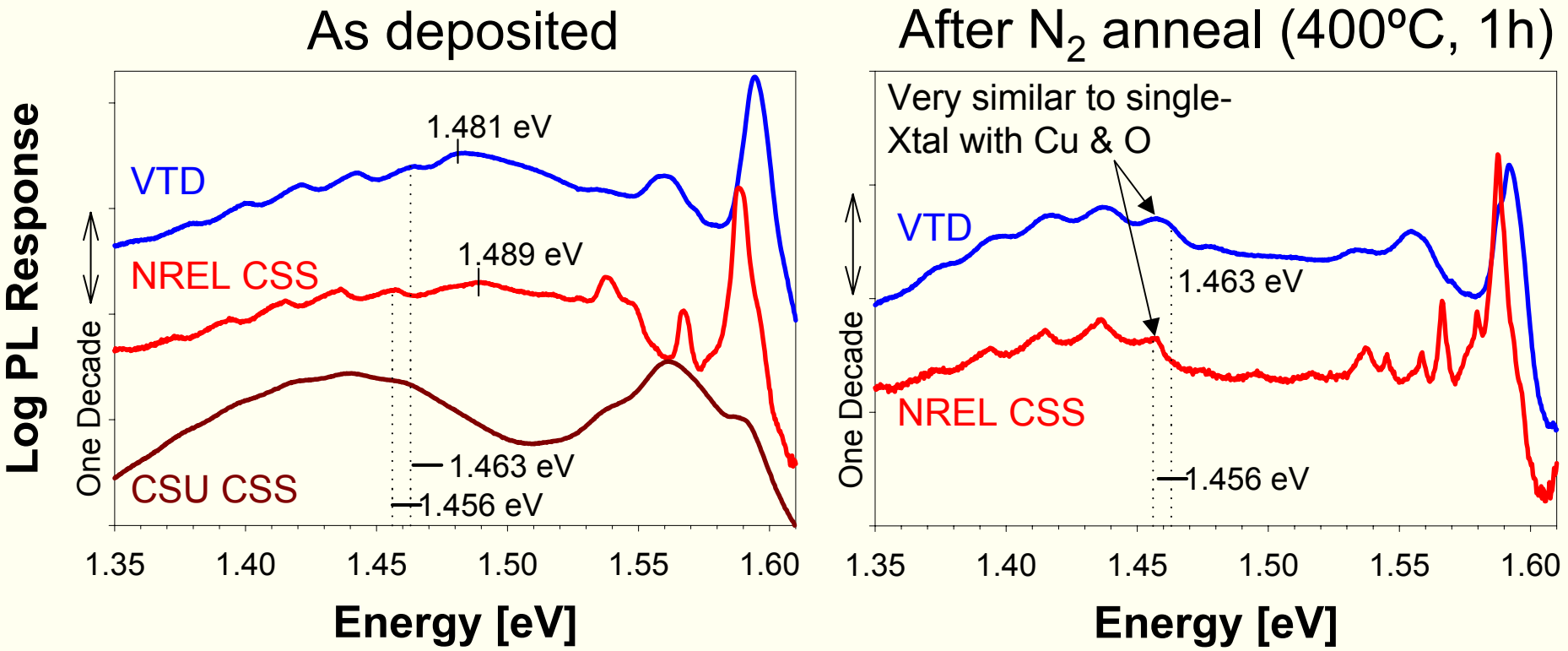


At 4.5 K
CdTe E_g = 1.606 eV



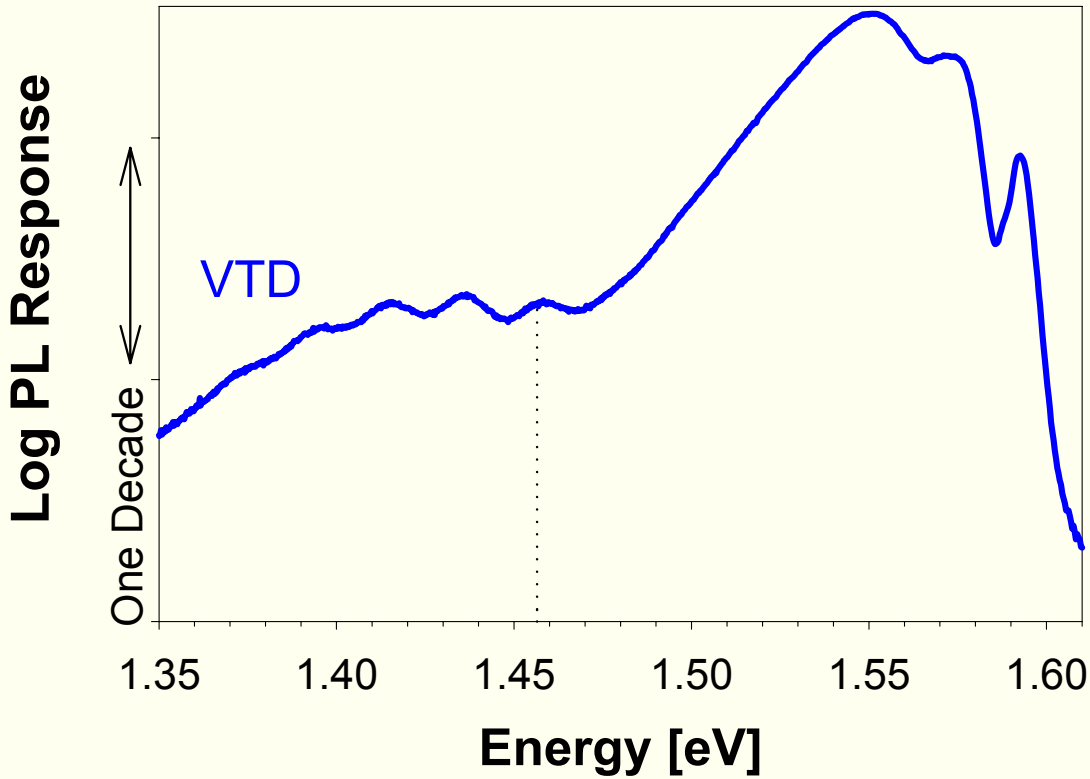
- 1.456-eV peak not intensity-dependent → Band-to-defect transition
- Defect energy ~ 150 meV

Thin-film CdTe: No $CdCl_2$



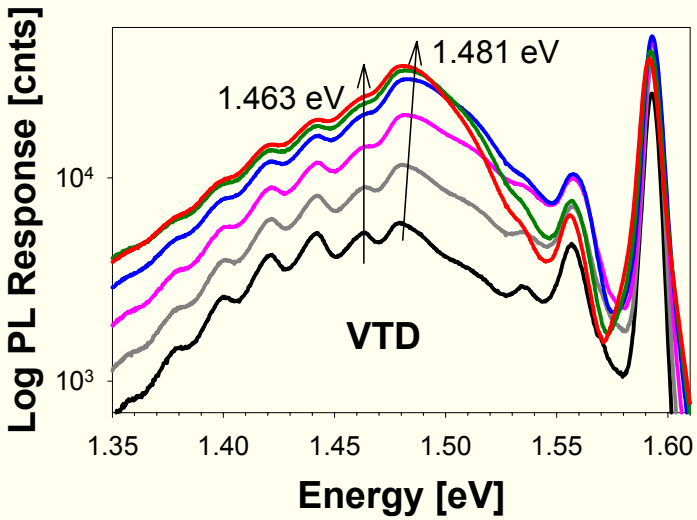
- All samples have a PL peak at ~1.46 eV
- VTD and NREL sample have peaks at 1.481 and 1.489 eV
- N_2 anneal eliminates 1.481- and 1.489-eV peaks

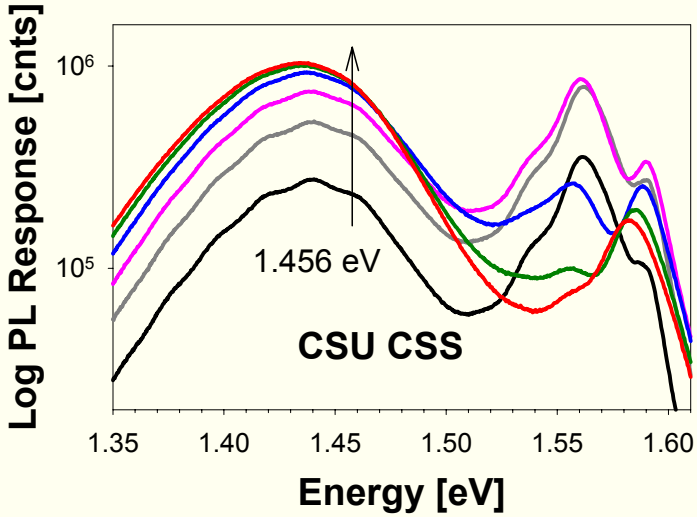
Thin-film CdTe: After $CdCl_2$

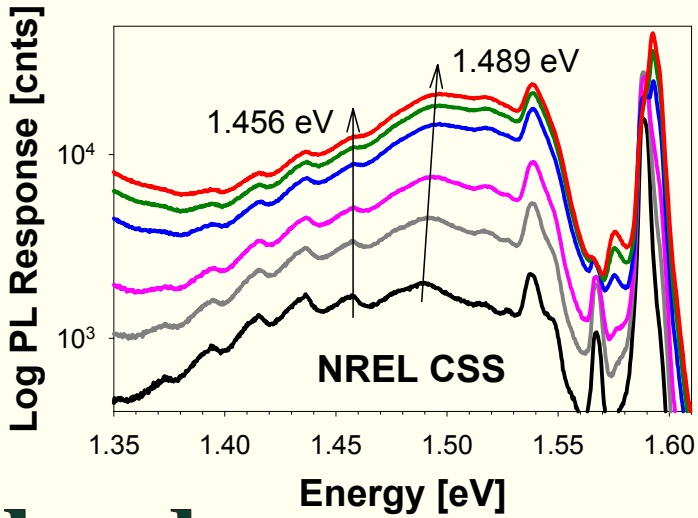


- VTD sample has PL peak at ~1.46 eV after $CdCl_2$
- New peak at 1.576 eV
- Peak at 1.55 eV brought out by $CdCl_2$ treatment

Intensity-dependent PL: Thin-film CdTe







- PL peaks at ~1.46 eV are intensity-independent → band to defect transition, defect energy ~ 150 meV
- PL peaks at 1.481 and 1.489 change → likely donor-acceptor transitions

Source of 1.456-eV Peak

Clues:

- Involves both Cu and O
- Defect energy of ~150 meV

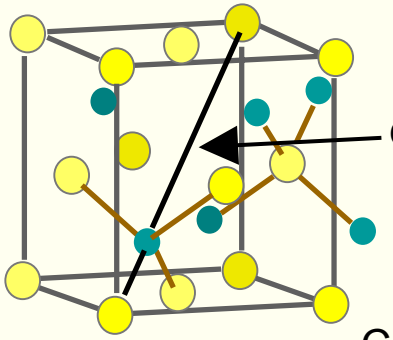
  Donor or acceptor level?

First principles band structure calculations:

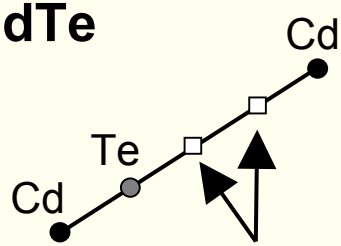
1. Defect-free CdTe
2. Only Cu in CdTe
3. Both Cu and O in CdTe

Theoretical Calculations (Li and Wei)

CdTe Lattice

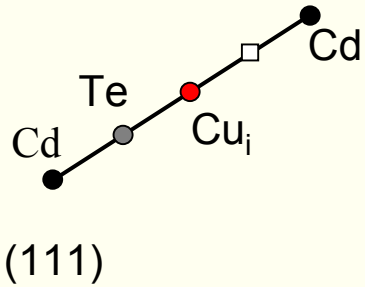


(I) CdTe



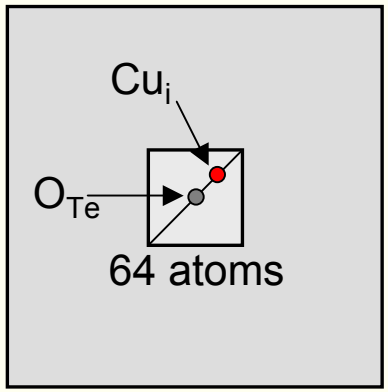
- Two points of low potential between the Cd and Te sites

(II) CdTe with Cu_i



- In p-type CdTe, Cu_i are more likely to form than Cu_{Cd}
- Cu_i prefer to sit next to the anion (Te) site

(III) CdTe with O_{Te}, Cu_i



- O_{Te} atom placed in the center of 512-atom supercell
- Cu_i initially placed next to the O_{Te} site and allowed to move within 64-atom cell

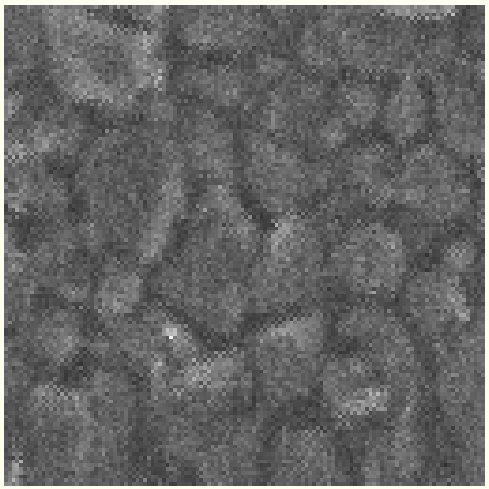
Results:

- Cu_i atom stays close to O_{Te} site
- Binding energy between O_{Te} and Cu_i is ~0.96 eV
- Activation energy of Cu_i-O_{Te} donor complex is ~125 meV

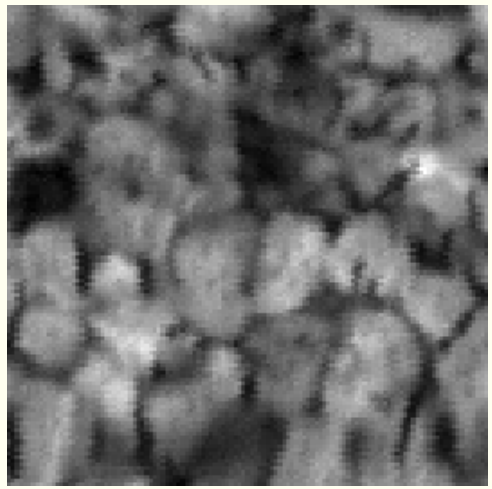
Cathodoluminescence Maps: NREL material (Romero)

Following $CdCl_2$ Treatment

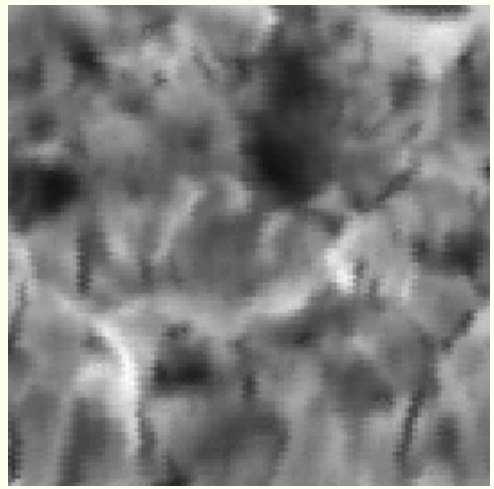
SEM



CL at 1.61 eV



CL at 1.46 eV



- 1.456-eV line appears to have non-uniform enhanced response at grain boundaries

Conclusions

- Single-crystal CdTe
  - 1.456-eV PL peak seen only when both Cu and O present
    - Intensity-independent → suggests band-to-defect transition, with defect energy of ~150 meV
- Thin-film CdTe
  - After deposition (no $CdCl_2$):
    - PL peaks at 1.456 eV (CSS) and 1.463 eV (VTD) intensity independent → band-to-defect transition
    - PL peaks at 1.481 eV (NREL CSS) and 1.489 eV (VTD) exhibit blue shift → DAP
  - After $CdCl_2$: VTD sample has intensity-independent peak at 1.456 eV
- Theoretical Calculations:
  - Cu_i-O_{Te} defect likely to form, donor level of ~125 meV
- CL Mapping Scans
  - Greater response of 1.456-eV line at some grain boundaries (non-uniform)