Effects of $CdCl_2$ treatment on the local electronic properties of polycrystalline CdTe measured with PEEM

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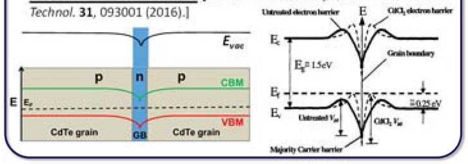
Introduction

Cadmium telluride (CdTe) is a polycrystalline photovoltaic (PV) material that has recently achieved power conversion efficiencies (21.5%) in research cells rivaling those of multicrystalline silicon. Further improvement of CdTe PV technology requires surpassing current limits in our understanding of fundamental mechanisms that influence processing-structure-property-performance relationships in CdTe. In particular, the influence of grain-boundary (GB) limitations and nano- or microscale nonuniformities have been identified as issues needing improved understanding.

CdTe GB models [Reviewed in J. D. Major, *Semicond. Sci. and Technol.* **31**, 093001 (2016).]



Objective & approach

- Objective: Determine processing-structure-property-performance-relationships critical for improving thin-film PV materials & devices
- Key Questions:

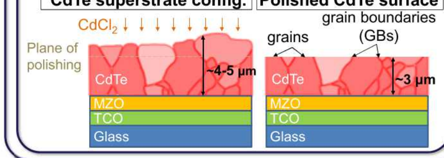
How does $CdCl_2$ treatment, a widely-used processing step, influence the local electronic structure of CdTe thin films?

Does oxygen (via air exposure) impact this step?

Sample preparation protocol

- NSG TEC 10 glass superstrates coated with transparent conducting oxide (TCO): $SnO_2/SiO_2/SnO_2$:F
- 100 nm $Mg_{0.23}Zn_{0.77}O$ (MZO) window layer
- 4-5 µm closed-space sublimation (CSS) CdTe
- CdTe films are mechanically polished
- Low-energy sputtering step: 50 eV Ar^+ ions / 10–20 min / ~0.1-0.15 µA•cm^{-2}
- Sample transfer with no additional air exposure by use of an inert gas (dry N_2) glove box
- X-ray Photoelectron Spectroscopy was used to verify surface composition after preparation steps

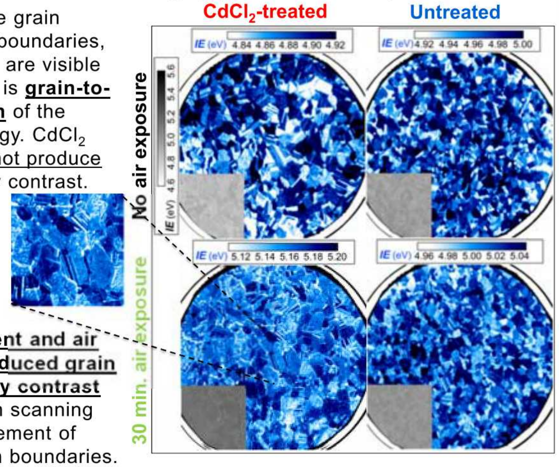
CdTe superstrate config.	Polished CdTe surface



Local ionization energy (PEY)

Take a set of images while sequentially varying the wavelength (λ). Extract an ionization energy (*IE*) value for each pixel.

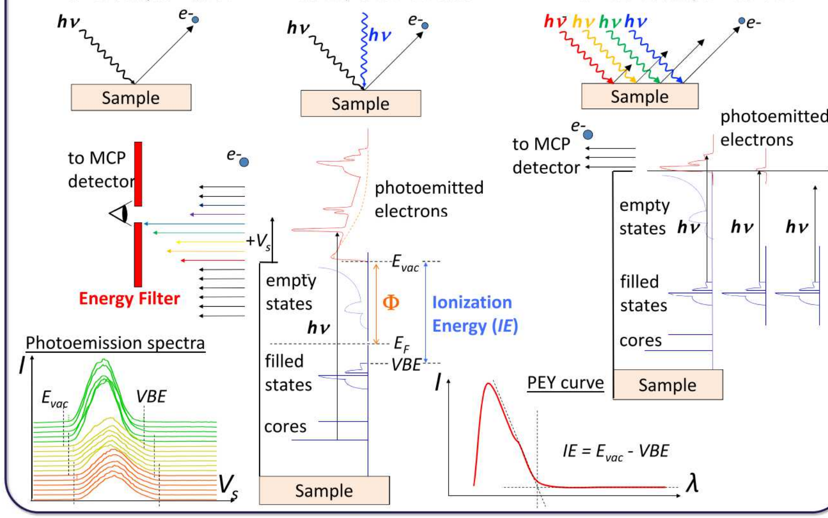
Microcrystalline grain domains, twin boundaries, & polish marks are visible in all maps, as is **grain-to-grain variation** of the ionization energy. $CdCl_2$ treatment did not produce grain boundary contrast.



$CdCl_2$ treatment and air exposure produced grain (GB) boundary contrast consistent with scanning probe measurement of activated grain boundaries.

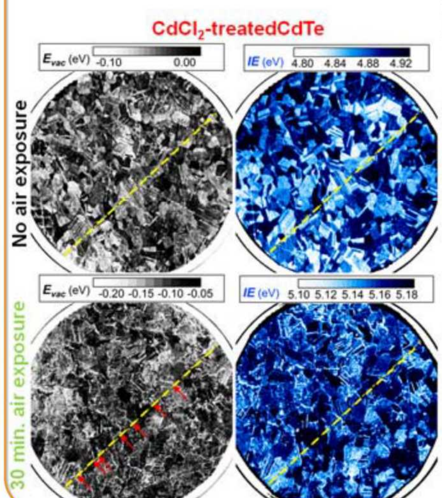
Oxygen increased the average ionization energy while $CdCl_2$ treatment decreased the average ionization energy.

Principles & methods: Spectroscopic PEEM

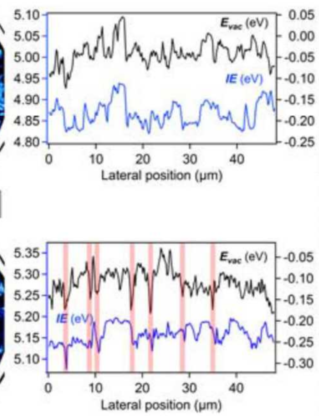


Local photoemission spectra (PES)

Take a set of images (stack) while sequentially varying the start voltage (V_s). Extract vacuum level cutoff (E_{vac}) threshold at each pixel.



Grain-to-grain variation of the vacuum level indicates work function variation. Vacuum level and ionization energy profiles track one another.



Grain-to-grain variation results in stepwise-like variation in the vacuum level and ionization energy profiles.

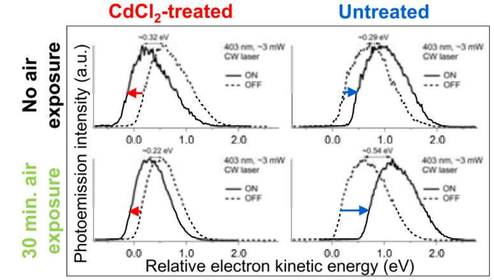
E_{vac} and *IE* profiles deviate after air exposure.

Dips in E_{vac} (red), consistent with GB downward bending suggested by scanning probe microscopy and electron-beam-induced current studies.

E_{vac}* + *IE decrease at GBs suggests a change in local chemical environment. Decrease in ***E_{vac}*** alone at GBs suggests electrostatic effects.

Surface photovoltage measurements

With and without additional illumination.



Additional illumination shifted E_{vac} to lower energy for $CdCl_2$-treated CdTe ⇒ upward surface band bending, while E_{vac} shifted to higher energy for untreated CdTe, indicating downward surface band bending.

The general model of SPV interprets the switch from downward to upward surface band bending as inversion from p-type to n-type.

Oxygen decreased/increased E_{vac} shifts for $CdCl_2$-treated/untreated CdTe. Along with ionization energy trends, this suggests that oxygen may passivate CdTe defects or perhaps act as a hole dopant.

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