

Diffusion Phenomena Related to Back Contacts in Thin-Film CdTe Solar Cells

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Thin-Film CdTe Solar Cells

- CdTe solar cells are generally superstrate devices.
- Module production is projected to surpass 1 GW/yr by 2010.
- Many fundamental properties of these devices are not fully understood, such as the role that Cu plays in back-contact formation.

Studies related to back-contact formation in CdTe solar cells:

- Temperature-reversible Cu_xTe surface phase precipitation
- Cu_xTe synthesis via Cu foil tellurization
- Pseudo-binary diffusion couple model applied to Cu migration in CdTe solar cells



The Role of Cu in CdTe Back-Contacts

CdTe forms a rectifying contact with most metals due to its high ionization potential, 5.7 eV.

Most back-contact schemes intentionally incorporate Cu to improve the contact.

Back-contact processes are empirically optimized, and Cu migration in the device has been implicated in some degradation mechanisms.



Cu ions : • - ON & • - IN the grains

K.D. Dobson, I. Visoly-Fisher, G. Hodes, and D. Cahen, Adv. Mater. **13**, 1495 (2001).

B. E. McCandless, J. E. Phillips, and J. Titus, Proc. 2nd WCPEC, 448 (1998).

Reaction Kinetics of Cu + CdTe



Thermal Desorption Mass Spectrometry (TDMS)

G. Teeter, J. Chem. Phys. **123**, 184713 (2005).

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Formation of Cu_xTe Phase at the Surface

Cu-doped CdTe(111)-B



XRD, XPS and AES indicate x ~ 2.

G. Teeter, J. Chem. Phys. 123, 184713 (2005).



Temperature-Reversible Cu_xTe Surface Precipitation: Cu-doped CdTe

X-ray Photoelectron Spectroscopy (XPS)



Observation:

At 300K, there is a substantial amount of Cu at the surface

At high temperatures, the Cu disappears



Temperature-Reversible Cu, Te Surface Precipitation: Cu-doped CdTe

Temperature-Programmed XPS



dT/dt = 2 K/min.

Hysteresis → nonequilibrium

Cu_xTe decreases \rightarrow Cu in-diffusion

We would like to model these data sets.



Effects of Surface-Precipitated Cu_xTe on Valence Electronic Structure



CdTe(111)-B substrate	SEC (eV)	VBM (eV)	IP (eV)
w/o Cu, T=325 K	15.98	0.45	5.69
w/ Cu, T>635 K	16.06	0.37	5.53
w/ Cu, T=325 K	16.38	0.00	4.84
Est. uncertainty	±0.03	±0.03	±0.06

Heavy Cu doping does not dramatically alter valence-band or IP.

Precipitated Cu_xTe lowers IP by about 0.9 eV.

Temperature-Reversible Cu_xTe Surface Precipitation: Cu-doped CdTe



Sample prior to TP-XPS •Cu + CdTe(111)-B •annealed to 675 K

Near-surface C_{Cu} about 10⁴ X bulk solubility

integrated Cu thickness = 11Å



Summary/Future Work

• Cu + CdTe \rightarrow Cu_xTe reaction kinetics

 observed T-reversible precipitation of Cu_xTe on CdTe surface with XPS

• UPS measurements show that surface Cu_xTe phase permits Ohmic-contact formation.

Quantitatively understanding this phenomenon requires a model that realistically couples near-surface bulk diffusion with surface phase separation.



