Rational Design of Wide Band Gap Buffer Layers for High-Efficiency Thin-Film PV

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SunShot BRIDGE (Bridging Research Interactions through Collaborative Development Grants in Energy)

1. Introduction

- Efficiency of production thin-film PV is significantly impacted by absorption in buffer layer (CdS)
- Higher performance wide band gap buffer material is needed

Objectives:
- Combine theory and characterization to enable optimization of new buffer materials
- Focus on defects & interfaces

Methods
- First-principles materials simulations of defect properties using hybrid functional DFT
- Atomic-scale imaging & compositional analysis using aberration-corrected scanning transmission electron microscopy
- World-class manufactured materials from MiaSolé Hi-Tech using all-PVD roll-to-roll process

2. Theoretical Basis of Effects of Point Defects, Band Alignments, and Fermi Level Pinning

Native Defects

- CdS-rich: Abundant donors
- Zn-rich: Vd- very favorable, 37% material very difficult
- CdS has near-ideal SCBM wet CVD/S
- ZnO CVD too high!
- ZnO CVD too low, but large opened in VBM
- (Cd,Zn)(0.08) can be ideal

CdS

ZnS

Growth-Related Impurities

O, H, & OH defects (PVD & CBD impurities)

C, N, & complexes w/ H (CBD impurities)

CdS

ZnS

Optical absorption from C-H defects is in the visible

CIGS

Deep levels from stable absorber-related defects

Intermixing

Migration Energy Barriers (eV)

Defect

Migration energy barriers (eV)

CIGS

CIGS

Band structure compared to CdS

3. Control of Film Deposition Characterized by STEM Imaging and EDS Analysis

Crystallinity

Lower O2 in process gas: Better epitaxy

"Standard" process: Mostly epitaxial buffer

Heterojunction Intermixing and Secondary Phases

Low O2 in PVD

High O2 in PVD

- Abrupt interface for S, Se, Ga (no mixing)
- Counter-doping of Cu & Cd across the CIGS/buffer interface may lead to buried pin-home-junction in CIGS

Cu-rich phase formation in buffer

Morphology depends on process conditions

High oxygen content suppresses Cu diffusion from CIGS, but enhances Zn diffusion from ZnO

4. Computational Optimization of Alloy Composition for High-Performance Buffer

Quaternary provides optimization degrees of freedom

Properties:
- Band gap
- Band offset
- Lattice match
- Dopability

- Targets: $E_g > E^\text{CdS}$, $-0.05 < \Delta E_{\text{CBO}} < 0.2$ eV; lattice match ±2.5%

Thermodynamic driving force for phase separation even at high T

Secondary phases are very stable: e.g. (Cd,Zn)Sx

5. Major Conclusions

- CdS is naturally favorable for its n-type dopability and favorable band alignment with CIGS
- ZnS is a BAD wide band gap buffer: $\Delta E_g$ too high, hard to n-dope, recombination centers from native defects
  $\Rightarrow$ But (Cd,Zn)(0,S) is a promising alloy system
- CIGS/buffer interface properties are critical and complicated
- Recombination affected by crystallinity
- Intermixing can bury p-n junction (Cd counter-doping)
- Intermixing can lead to unfavorable secondary phases (Cu in CdS)
- Sputter deposition conditions, particularly oxygen in process gas, can control quality and composition of interface region
- Careful selection and optimization of buffer material is dependent on absorber material

References:


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