Passivating the Grain Boundaries in CdTe: A First-principles Study

Chuan-Jia Tong
04/01/2018
Department of Physics, University of York
1 Background

2 Simulations on CdTe GBs

3 Conclusion
Background

Humanity’s Top Ten Problems for next 50 years

1. ENERGY
2. WATER
3. FOOD
4. ENVIRONMENT
5. POVERTY
6. TERRORISM & WAR
7. DISEASE
8. EDUCATION
9. DEMOCRACY
10. POPULATION

2003 6.3 Billion People
2050 8-10 Billion People
CdTe

Zinc Blende

Band Structure

Lattice Constants

\[ a=b=c=6.48 \text{ Å} \]

Band-gap

1.45~1.55 eV

CdTe cell

Glass

Transparent conductive oxide

CdS layer

CdTe absorb

Metallic back contact

Current
Grain Boundaries in CdTe

Recombination by grain-boundary type in CdTe

John Moseley,1,2,a Wyatt K. Metzger,1 Helio R. Moutinho,1 Naba Paudel,3 Harvey L. Guthrey,1 Yana Yan,3 Richard K. Ahrenkiel,1,2 and Mowafak M. Al-Jassim1

1National Renewable Energy Laboratory, 15013 Denver West Parkway, Golden, Colorado 80401, USA
2Colorado School of Mines, 1500 Illinois Street, Golden, Colorado 80401, USA
3Department of Physics & Astronomy, University of Toledo, Toledo, Ohio 43606, USA


would introduce trapping states and non-radiative recombination centers.

It probably stems from the impurities
Possible effects of oxygen in Te-rich Σ3 (112) grain boundaries in CdTe

Chunbao Feng a,b,c, Wan-Jian Yin d, Jinlan Nie a, Xiaotao Zu a, Muhammad N. Huda b, Su-Huai Wei c, Mowafak M. Al-lassim c, Yanfa Yan d,e

Study of photoelectrochemical properties of polycrystalline CdTe thin film solar cells

View
1 Background

2 Simulations on CdTe GBs

3 Conclusion
Methods

Approach: Density Functional Theory (DFT)

Software: VASP

Functional: PBE, HSE06 (for some SCF calculations)
Four Grain Boundaries

$\Sigma 3 \, (111)$

$\Sigma 3 \, (112) \text{ Te core}$

$\Sigma 3 \, (112) \text{ Cd core}$

$\Sigma 5 \, (310)$

Bulk-like

GB

GB

GB
1. No gap state in $\Sigma^3$ (111)
2. One deep gap state in $\Sigma^3$ (112) Te core
3. One shallow gap state in $\Sigma^3$ (112) Cd core
4. One deep and one shallow gap state in $\Sigma^5$ (310)
1. No segregation behavior in $\Sigma 3$ (111)
2. Almost no segregation behavior in dopant Se
3. All dopants (except for Se) prefer segregating to GB
4. Cl and Na have a strong tendency to break down dangling bonds
The anion dopants can eliminate gap states by breaking down the dangling bonds.
Cl_{Te} can eliminate the deep gap state induced by Te-Te dangling bond, \( \text{Na}_{\text{Cd}} \) can eliminate the shallow gap state induced by Cd-Cd dangling bond.
The position of gap state is determined by the dangling bond length of O-Te.
Cl, Na co-doping can remove all gap states in GB $\Sigma 5$ (310), which is helpful to whole performance.
1 Background

2 Simulations on CdTe GBs

3 Conclusion
1. GB $\Sigma 3$ (111) is the most stable and clean one.

2. All extrinsic dopants except for Se prefer segregating to GB.

3. $O_{Te}$ can only passivate the long Te-Te DB, $Cl_{Te}$ can passivate both long and short Te-Te DB, $Na_{Cd}$ can break down Cd-Cd DB.

4. $Cl$, $Na$ co-doping can effectively passivate all GBs in CdTe.
Acknowledgement