Voc impact of orientation-dependent x in anisotropic PV absorbers

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Accessibility
$V_{OC}$ impact of orientation-dependent $\chi$

in anisotropic PV absorbers

Rupak Chakraborty$^1$
David Berney Needleman$^1$, Kelsey Doolittle$^1$, Niall M. Mangan$^1$, Vera Steinmann$^1$, Jeremy R. Poindexter$^1$, Alex Polizzotti$^1$, Chuanxi Yang$^2$, Roy G. Gordon$^2$, and Tonio Buonassisi$^1$

$^1$Massachusetts Institute of Technology
$^2$Harvard University

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$V_{OC}$ deficit in SnS

- Many PV material systems are plagued by low $V_{OC}$
- CZTS, WS$_2$, FeS$_2$, SnS

\[ V_{OC}^{\text{deficit}} = \frac{E_g}{q} - V_{OC} \]

\[ = 728 \text{ mV} \]

What causes low $V_{OC}$?

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Band fluctuations: constant $\chi$

- $V_{OC}^{\text{defic}}$ significantly influenced by electrostatic potential fluctuations$^{1,2}$

\[ E \]
\[ E_v \]
\[ E_c \]
\[ E_{\text{vac}} \]

\[ \chi \text{ constant} \]
\[ E_g \text{ constant} \]

\[ \sim 10 \text{ meV} \]

$^{1,2}$J.H. Werner et al., Thin Solid Films 480-481, 399 (2005).
$^{1,2}$Gokmen et al., Applied Physics Letters 103 (2013)
Band fluctuations: variable $\chi$

$E$ vs. position:
- $E_{vac}$
- $E_c$
- $E_v$
- $\chi$ variable
- $E_g$ constant
- $\sim 100$ meV
Surface orientation dependence of electron affinity

\[ \Delta \chi = \chi_{hkl} - \chi_{h'k'l'} \]

Max measured \( \Delta \chi \) (eV)

- Si \(^1\)
- CuGaSe\(_2\) \(^2\)
- GaAs \(^3\)
- In\(_2\)O\(_3\) \(^4\)

Lateral CBO variation due to grain orientation

What is the impact of orientation-dependent electron affinity on SnS device performance?
Simple test case: two-grain model

Single stack previously modeled in SCAPS 1D

\(^1\text{Mangan et al., J. Appl. Phys. 118, 115102 (2015).}\)
Electron affinity parameter space

\[ \chi_1 \text{ (eV)} \]

\[ \chi_2 \text{ (eV)} \]

\[ \Delta \chi = 0 \text{ eV} \]

\[ \Delta \chi = 0.9 \text{ eV} \]
Efficiency impact

\[ \chi_1 \text{ (eV)} \]

\[ \chi_2 \text{ (eV)} \]

\[ \eta \text{ (%)} \]

Optimal \( \eta \)
$V_{OC}$ impact

$\chi_1$ (eV)  $\chi_2$ (eV)  $V_{OC}$ (V)

Optimal $\eta$

Cliff offset

Cliff offset
$J_{SC}$ impact

$$J_{SC} \text{ (mA/cm}^2\text{)}$$

$\chi_2 (\text{eV})$

$\chi_1 (\text{eV})$

Optimal

Spike offset

Spike offset

$\eta$
Efficiency impact

\[ \eta_2 (\text{eV}) \]

\[ \eta_1 (\text{eV}) \]

\[ \eta \] (\%)

Optimal

1.1% absolute
22% relative loss

Current blocking
Summary

- Abrupt lateral fluctuations in $\chi$ are expected in SnS due to orientation dependence
- Current blocking is worst effect
  - Avoided by optimizing buffer layer
  - $V_{OC}$ still reduced because of cliff offset
  - 22% relative loss in efficiency for $\Delta\chi = 0.9$ eV
Further work

- Confirm $\chi(hkl)$ in SnS experimentally
- >2 grains in parallel
Further work

- Confirm $\chi(hkl)$ in SnS experimentally
- >2 grains in parallel
- Simulation accounting for 2D carrier flow
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\[ \chi_1 (eV) \]

\[ \chi_2 (eV) \]

Current blocking

Optimal \( \eta \)

1.1% absolute

22% relative loss

Current blocking

\( \eta \) (%)