Research Center for Photovoltaics

Investigation of TiO_x as carrier selective contact for crystalline silicon solar cells

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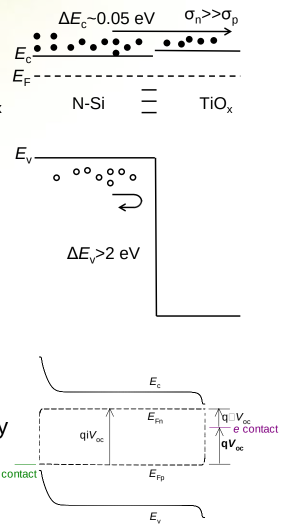
Motivation

- TiO_x (TiO_2) electron contact by thermal-ALD provides η=21.6% (ANU) [1].
- In general discussion, electron selectively of TiO_x originates from the asymmetric band offset at the N-Si/TiO_x interface [1,2].
- Nevertheless, it was suggested that TiO_x contains negative fixed charge [3,4], which might be detrimental for electron contact.



Research objective / open issues
-Is selectivity simply determined by band alignment?
-Is c-Si band bending induced by TiO_x?
-Carrier selectivity should be evaluated independent of surface passivation quality (e.g., external V_{oc} vs iV_{oc}) [5].

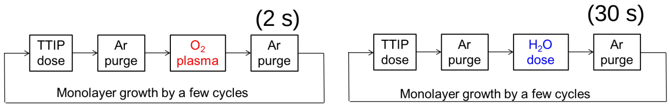
[1] X. Yang *et al.* Adv. Mater. **28**, 5891 (2016).
[2] S. Avasthi *et al.* Appl. Phys. Lett. **102**, 203901 (2013).
[3] B. Liao *et al.* Appl. Phys. Lett. **104**, 253903 (2014).
[4] J. Cui *et al.* SOLMAT **158**, 115 (2016).
[5] M. Bivour *et al.* IEEE JPV **4**, 566 (2014).

In this work, carrier selectivity of ALD-TiO_x layers is investigated by measuring external V_{oc} of the test solar cells [6].

[6] T. Matsui *et al.* presented at Silicon PV (Freiburg, 2017) and submitted.to Enegy Procedia.

TiO_x by atomic layer deposition (ALD)

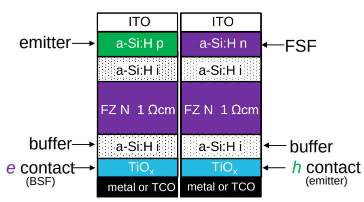
- Titanium precursor: TTIP (Titanium tetraisopropoxide)
- Oxidation : plasma (O_2) or thermal (H_2O)
- Similar growth rate (~0.045 nm/cycle) for both ALD processes
- However, substantially longer t_{purge} needed for thermal (>30 s) than for plasma (2 s)
- Refractive index differs slightly (plasma: n=2.40, thermal: n=2.32 @λ=632 nm).



plasma-ALD thermal-ALD

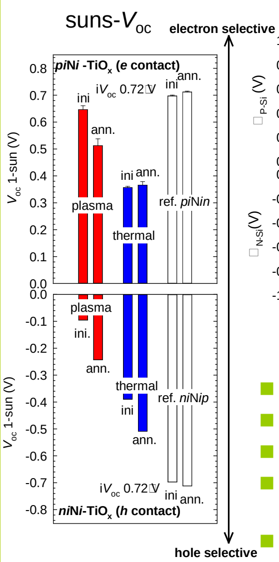
Sample structures and characterization

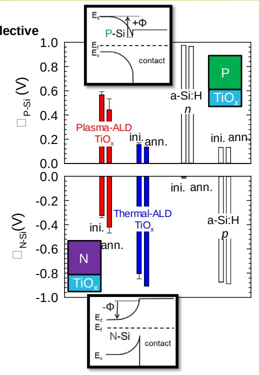
TiO_x as rear contacts in solar cell precursors

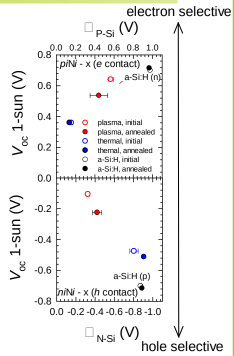


- a-Si:H (i) buffer between Si and TiO_x
- 6-nm-thick TiO_x deposited by plasma- or thermal-ALD at rear
- TiO_x either as *e* contact (BSF) or *h* contact (rear emitter)
- Various capping materials (Ti, Al, ITO, Pd) examined on top of TiO_x
- Front emitter and front-surface-field (FSF) by a-Si:H heterojunction (p-i , n-i)
- Suns-V_{oc}, Surface photovoltage (SPV), QSSPC

Suns-V_{oc} and SPV measurements



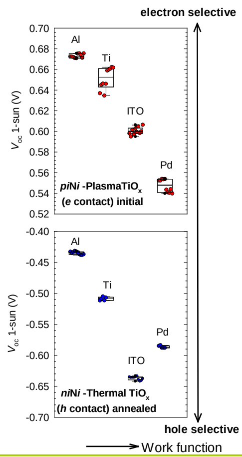




TiO_x/Ti contact

- V_{oc} (1-sun) as a measure of carrier selectivity
- Plasma-ALD TiO_x : electron selectivity
- Thermal-ALD TiO_x : hole selectivity
- Post-annealing declines electron selectivity but enhances hole selectivity.
- Inverse polarity of induced c-Si band bending (Φ) by two ALD processes even using the same precursors
- Correlation found between Φ and selectivity

Influence of metal (TCO) contact



- Carrier selectivity is significantly influenced by the work function (WF) of capping layer material (Ti: 4.3 eV, Al: 4.2 eV, Pd: 5.4 eV [7], ITO: 4.8 eV [8]).
- Improved electron contact by TiO_x/Ca (WF<3 eV) has been reported [9].
- Screening length of TiO_x is well above the thickness.
- As a result, carrier selectivity can be tuned from electron (V_{oc}~680 mV) to hole selective (V_{oc}~650 mV).

[7] CRC Handbook of Chemistry and Physics (92nd ed.) 12-124.
[8] A. Klein *et al.* Thin Solid Films **518**,1197 (2009).
[9] T. G. Allen *et al.* Proc. 43rd IEEE PVSC 230 (2016).

Summary

- TiO_x layers were deposited by plasma- and thermal-ALD.
- Inverse behavior in terms of carrier selectivity/induced c-Si band bending
  - Plasma ALD: electron selective contact
  - Thermal ALD: hole selective contact
- Carrier selectivity is widely tunable from electron selective (V_{oc} ~680 mV) to hole selective (V_{oc} ~650 mV), depending on ALD process, post annealing and WF of metal (TCO) contact.
- It suggests that carrier selectivity is governed by the effective work function and/or the fixed charge of TiO_x rather than by the asymmetric band offsets at the Si/TiO_x interface (induced-junction-like classical MS/MIS).
- Strong influence of capping layer might be an issue for realizing high-η device (e.g., TiO_x/TCO/metal *e* contact).

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