Atomic layer deposited Indium oxy-sulfide on CZT(S,Se) absorbers

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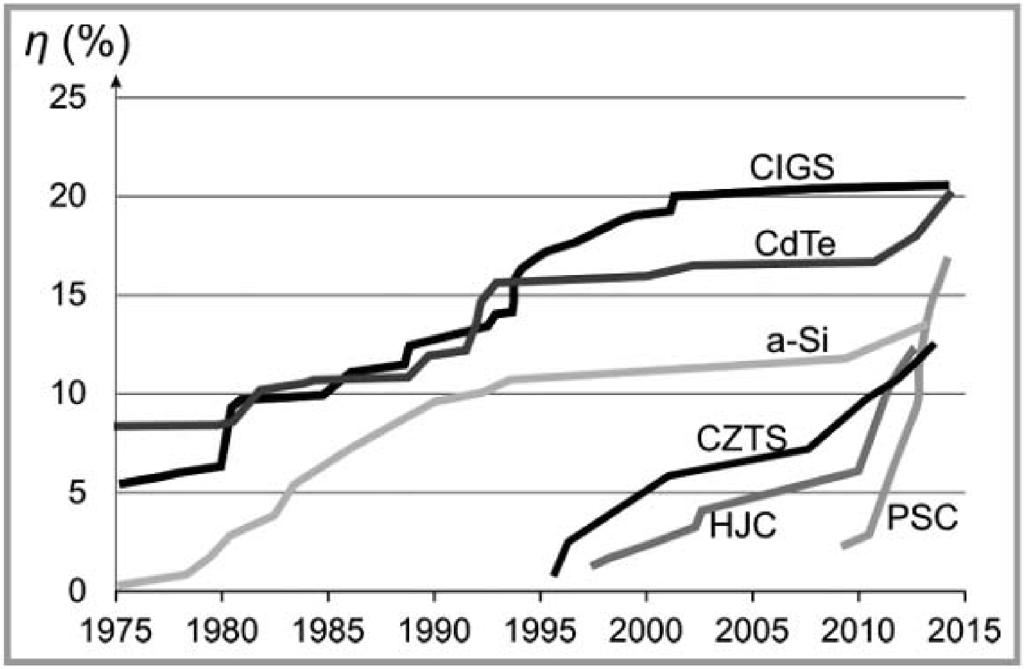
Outline

- Motivation
- ALD of In_2S_3 thin films
- Band alignment studies and need for $In_2(O,S)_3$
- ALD of In_2O_3 thin films
- Tuning S:O ratio in $In_2(O,S)_3$
- Summary

Relative progress of CZTS Solar Cell Efficiency



Research Cell Efficiency Records,
NREL, Golden, CO. www.nrel. gov/ncpv/

Strategies for higher efficiency:

- More stable buffer layer than CdS to avoid interdiffusion
- More reflective back contact to increase current
- Lower recombination at back contact to increase voltage

Why Replace CdS buffer with $In_2(O,S)_3$?

Problems with Chemical bath deposited (CBD) CdS

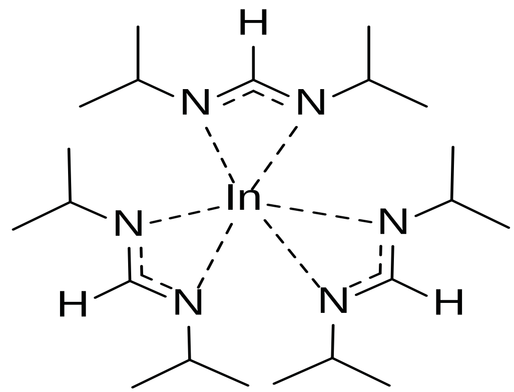
- Toxicity of Cadmium
- Presence of uncontrolled oxygen content
- In a superstrate configuration Cd^{2+} ions diffuse during high-temperature anneal

Solution: Atomic Layer Deposited (ALD) S:O tunable $In_2(O,S)_3$

- Non-toxic $In_2(O,S)_3$ can have good band alignment with CZTS[1]
- Control over in-situ Oxygen content => tunable conduction band offset
- Diffusion of In^{3+} is slower than Cd^{2+}, enabling a superstrate configuration with a more efficient back contact made as the last step

(1)Barkhouse *et*.al. – App. Phys. Lett. 100, 193904 (2012)

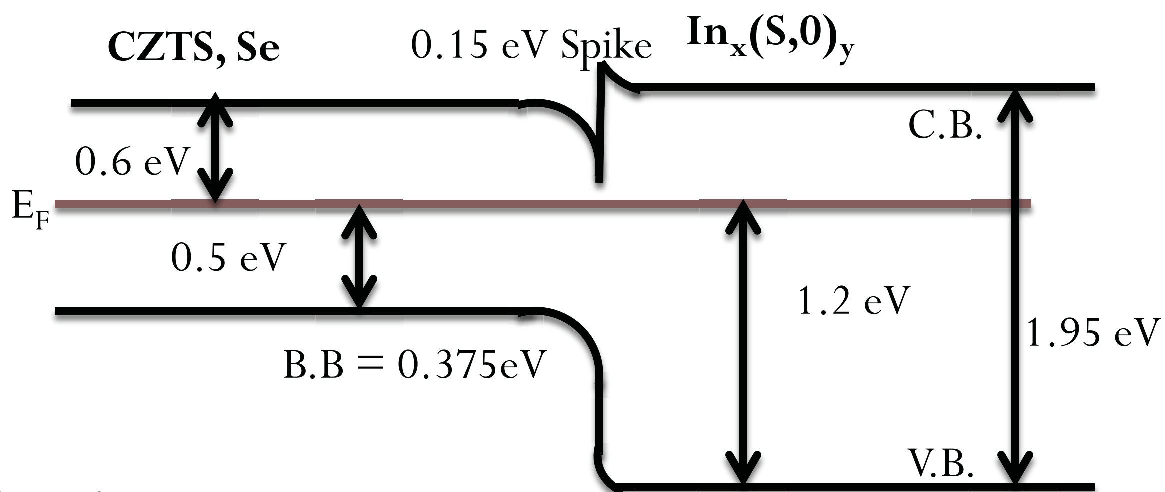
A new indium formamidinate precursor with H_2S provides low-temperature, carbon-free ALD of In_2S_3

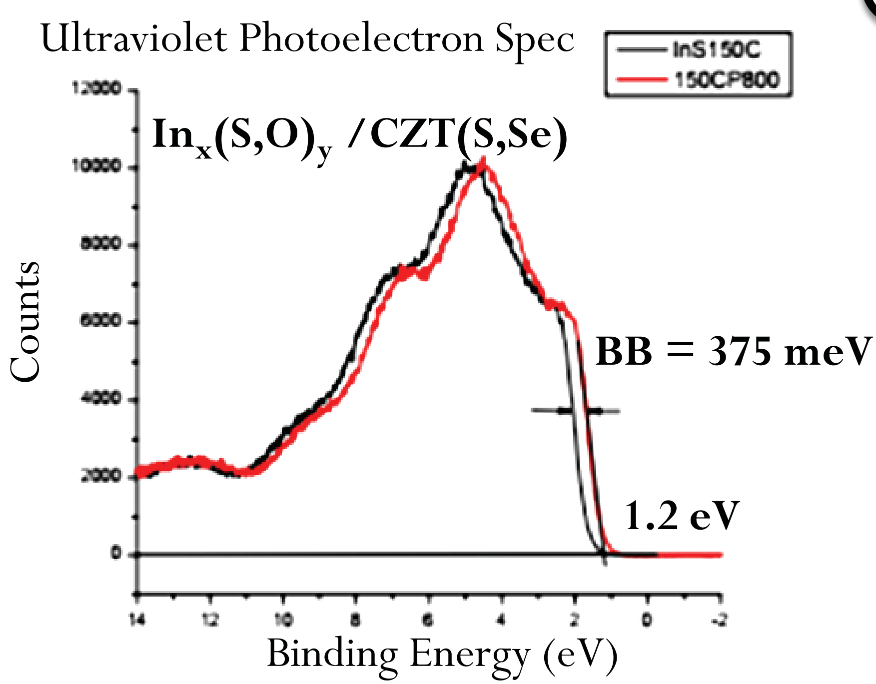


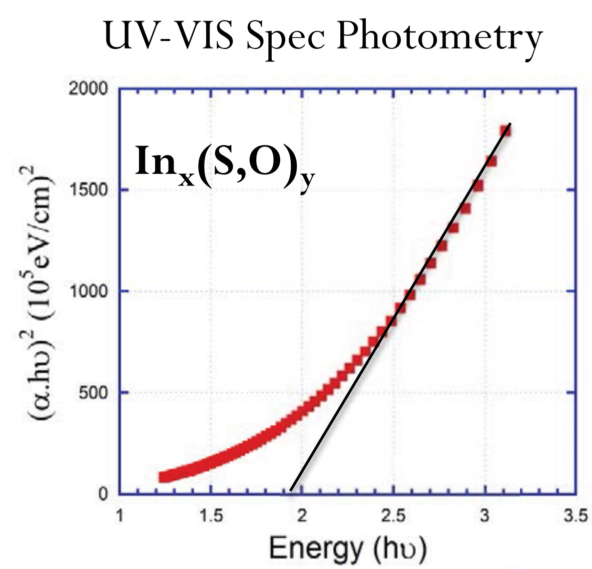
Newly synthesized tris(*N,N'*-diisopropylformamidinato)indium precursor vaporized at 130 °C

ALD In_2S_3 films grow at 0.65 A°/cycle on substrates at 150 °C have negligible contamination by carbon, nitrogen or oxygen

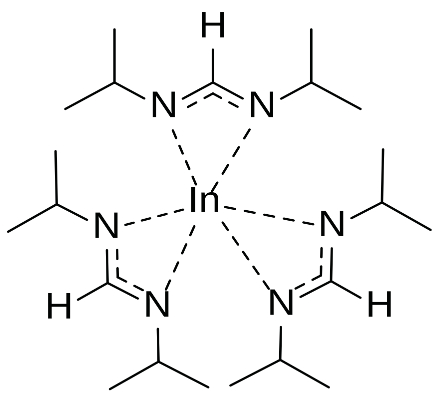
ALD provides $In(S,O)_3$ with good band alignment (oxygen results from post-ALD diffusion)





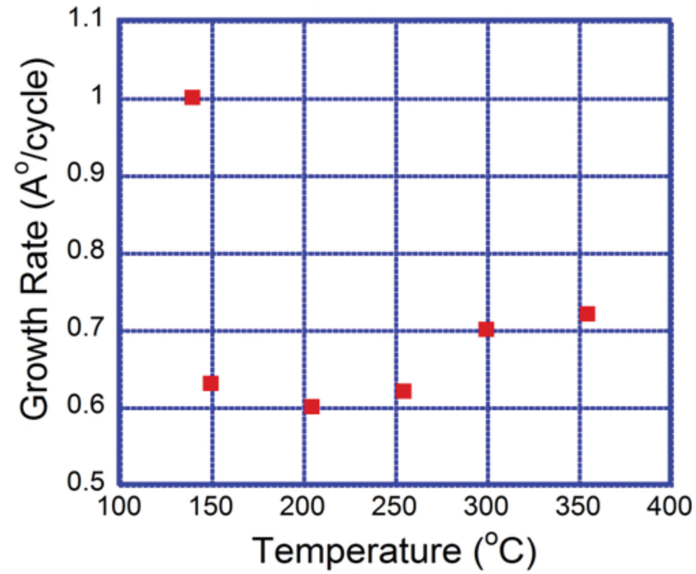


ALD In_2O_3 from indium formamidinate and H_2O



tris(*N*,*N*'- diisopropylformamidinato)indium

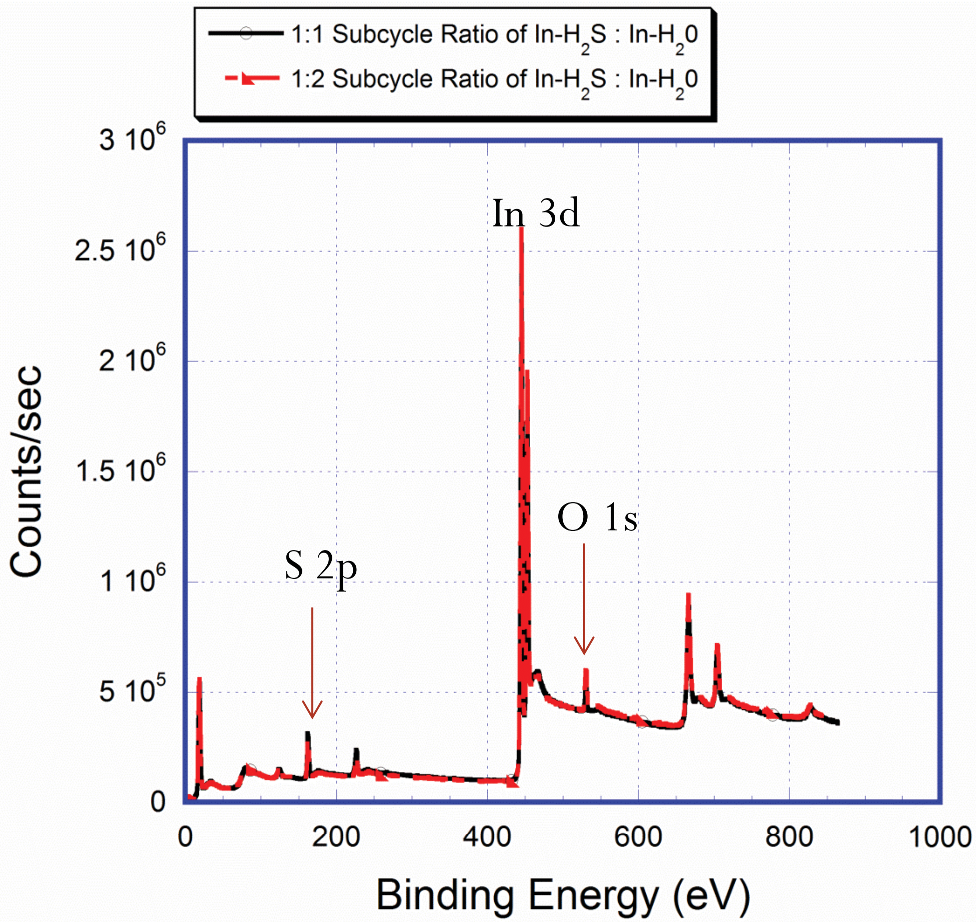
Indium oxide ALD growth window using a newly synthesized, highly volatile indium formamidinate precursor (1) .



✓Low carbon (which contaminated $In_2(acac)_3$ films), no oxygen or nitrogen contamination

✓Reduced copper diffusion during ALD (in substrate configuration), because deposition time is shorter than with $In_2(acac)_3$

ALD of ternary $In_2(O,S)_3$ with tunable S:O



X-Ray Photoelectron Spectroscopy Results

Element	Atomic % after ~ 120 sec Ar etch	
	1:1 In-H_2S to In-H_2O Ratio	1:2 In-H_2S to In-H_2O Ratio
In	43.2	43.1
S	36.2	28.3
O	20.6	28.6
C	< 1%	< 1%
N	< 1%	< 1%

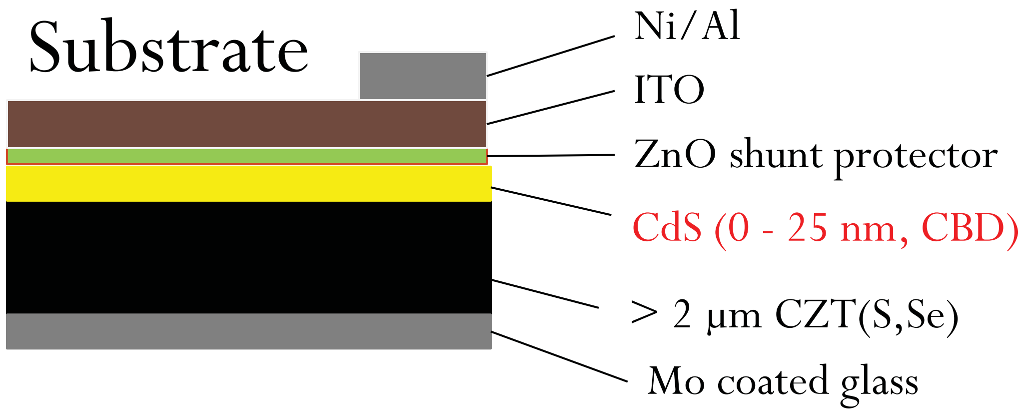
ALD at 210 °C substrate temperature

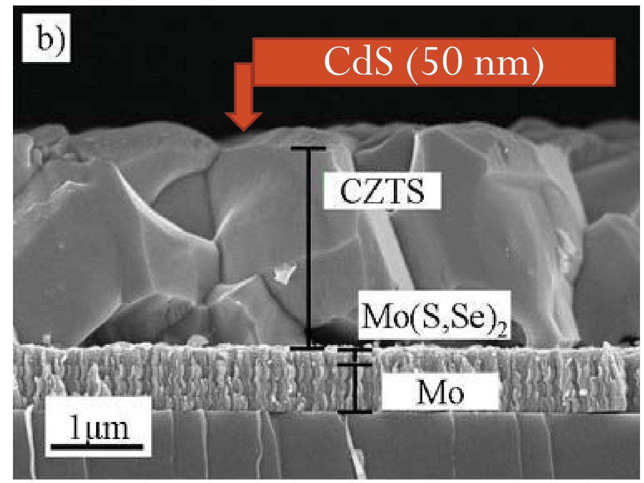
Indium Formamidinate-H_2S cycle followed by Indium Formamidinate-H_2O

Reactivity of Indium Formamidinate with H_2S roughly twice that of H_2O

Motivation to target Superstrate v/s the Substrate Configuration for CZT(S,Se) Cells

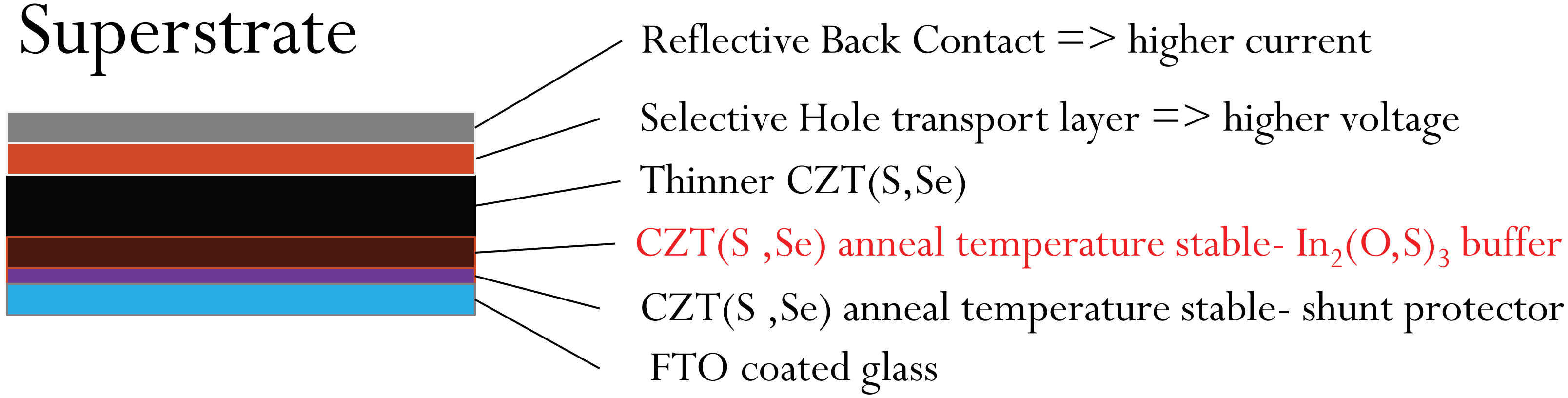
Substrate





Wang *et*. al. – Advanced energy Materials 2014, 4, 1301465

Superstrate



Summary

- ALD process conditions for pure, stoichiometric In_2S_3, In_2O_3 and $In_2(O,S)_3$
- $In_2(O,S)_3$ with high sulfur content identified as a promising choice for non-toxic buffer on CZTS,Se absorber with ideal conduction band offset
- ALD process for tunable S:O in $In_2(O,S)_3$ established

Thanks for your attention!

Acknowledgements

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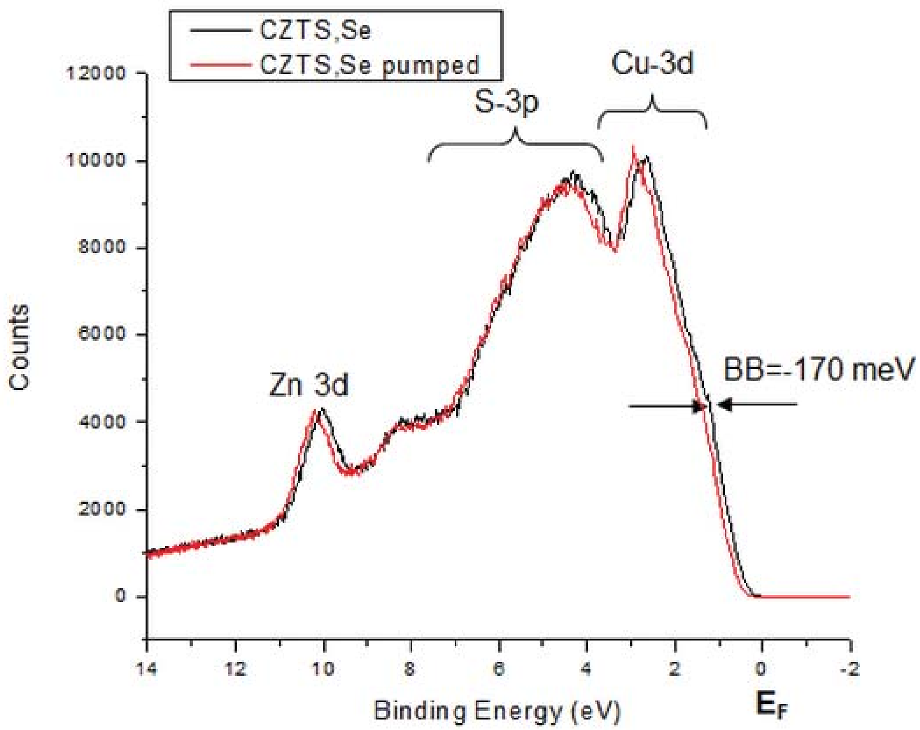

Blowup of band edge region CZTS,Se