Master’s Thesis Engineering Technology

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Best suited device architectures and selective contacts for thin film Van der Waals materials based on Sb_2Se_3 chalcogenide and SbSeI chalcohalide compounds

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1 Introduction

Thin film solar cells have become a hot topic for their interesting applications in building integrated photovoltaics (BIPV) and the possibility to achieve higher efficiencies with multi-junction devices by combining them with existing PV technologies. A big focus lays on the development of these technologies from environmentally friendly materials to ensure safety and sustainability. chalcohalide, like antimony selenide (Sb_2Se_3) and antimony selenoiodide (SbSeI), share these advantages and shows useful wide bandgap properties for PV applications.

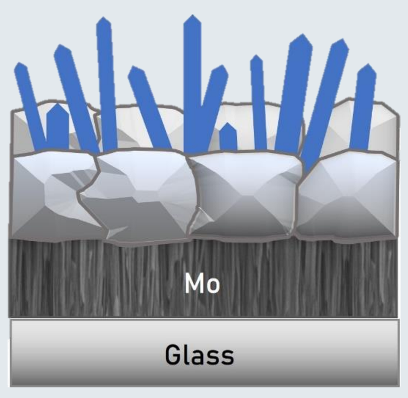

Fig. 1 Substrate with SbSeI structures.

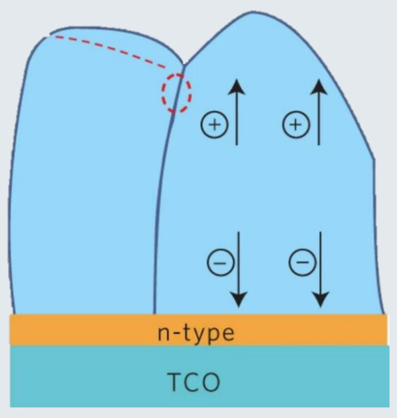

Fig. 2 Substrate with Sb_2Se_3 structures [1].

2 Device synthesis

SbSeI is an emerging thin film material and has limited research on device architecture and electron/hole selective contacts. This master’s thesis will mainly be focused on the synthesis of different possible device configurations and selective contacts by comparing them to a reference absorber material like Sb_2Se_3. This is achieved by using proven materials as selective contacts.

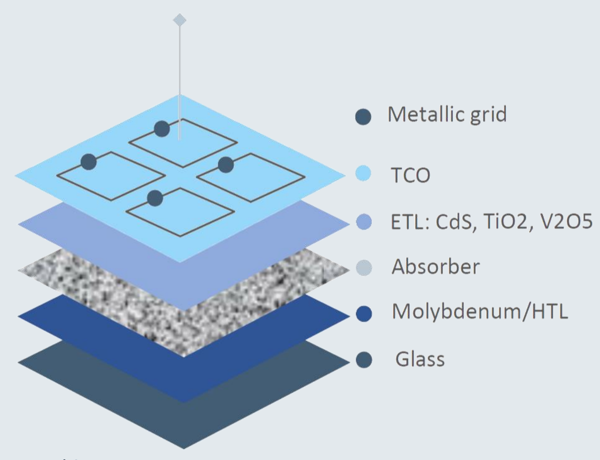

Fig. 3 Substrate configuration [1].

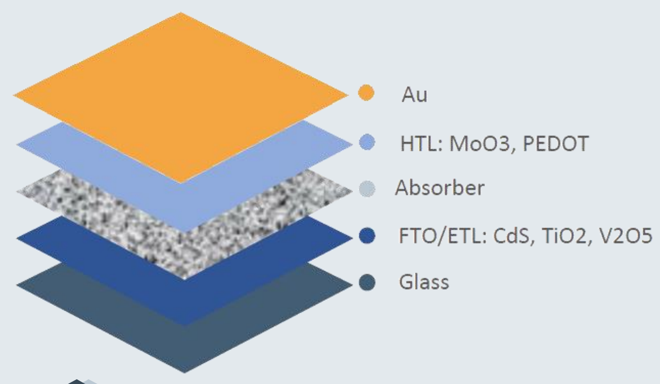

Fig. 4 Superstrate configuration.

Deposition techniques:
- Sputtering
- Thermal evaporation
- Annealing
- Spin coating
- Atomic layer deposition (ALD)
- Chemical bath deposition (CBD)

Contact materials:

ETL’s:
- Cadmium sulfide (CdS)
- Titanium dioxide (TiO_2)
- Vanadium pentoxide (V_2O_5)

HTL’s:
- Molybdenum (Mo)
- Molybdenum trioxide (MoO_3)
- PEDOT

Fig. 5 Co-evaporation and sputtering equipment (top), CBD (right) and low-pressure annealing (left).

3 Characterization results

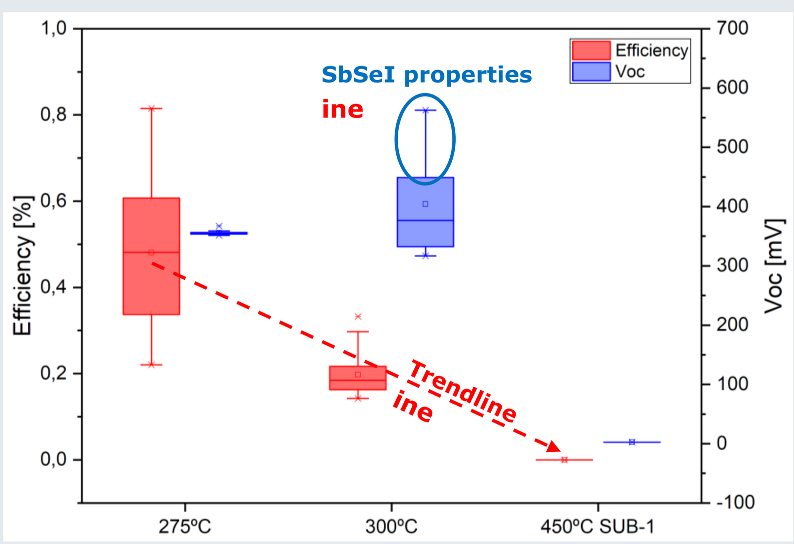

Fig. 6 Efficiency and V_{oc} to annealing temperature.

- SbSeI devices show no response
- Trendline visible with previously synthesized devices at different annealing temperatures
- Increasing annealing temperature decreases device efficiency

- Sb_2Se_3 device XRD angles match with experimental pattern, intensities not so much
- SbSeI device XRD angles and intensities show high similarity to experimental pattern

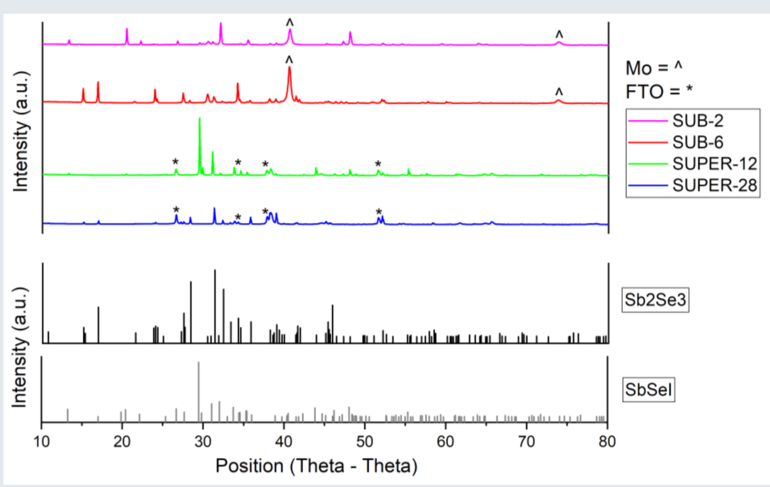

Fig. 7 X-ray Diffractogram (XRD) from synthesized devices and experimental patterns from Sb_2Se_3 and SbSeI.

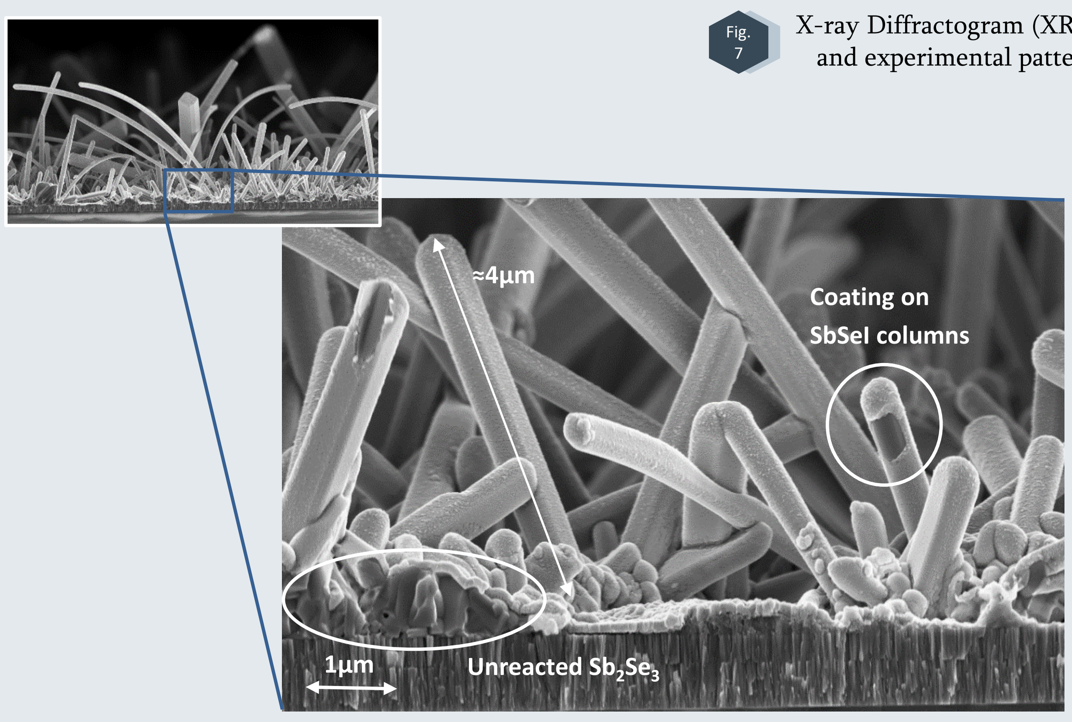

Fig. 8 Cross sectional SEM image of SbSeI device.

- Presence of unreacted precursor
- Large columns up to 10’s of micrometers
- Bad absorber layer coverage

4 Conclusion

- SbSeI absorber layers do not really form thin films and show a very uneven surface morphology making the deposition of contact layers difficult
- More precursor reacts with increasing annealing temperature worsening absorber coverage due to column like structures which leads to an increase in shunt paths
- Diffractograms from devices with SbSeI show similarities to experimental pattern based on powder, indicating non-uniform crystalline orientation
- Columnar structures seem to be very fragile to external forces, broken due to centrifugal forces that occur during spin coating

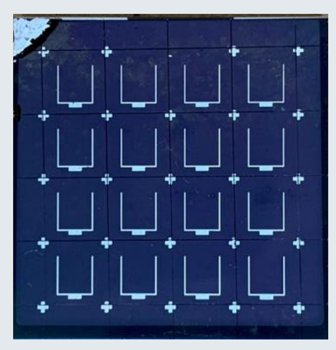

Fig. 9 Finished substrate device containing SbSeI absorber.

- Future work could focus on minimizing column heights and maximizing layer coverage and strength. Introducing a type of passivation layers might reduce shunt phenomenon.

Supervisors / Co-supervisors / Advisors: Prof. Dr. Edgardo Saucedo (UPC), Prof. Dr. Bart Vermang (UHasselt/Imomec)

References: [1] K. Zeng, D.-J. Xue, and J. Tang, “Antimony selenide thin-film solar cells,” Semiconductor Science and Technology, vol. 31, no. 6, p. 063001, Apr. 2016, doi: 10.1088/0268-1242/31/6/063001.

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