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Over 10μm grain size Sb_2Se_3 film and its effective surface passivation

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Outline

1. Superstrate: Large grain size film deposition
2. Substrate: Effective surface passivation method
3. Acknowledgements

Various advantages of Sb_2Se_3

Commercial prospect

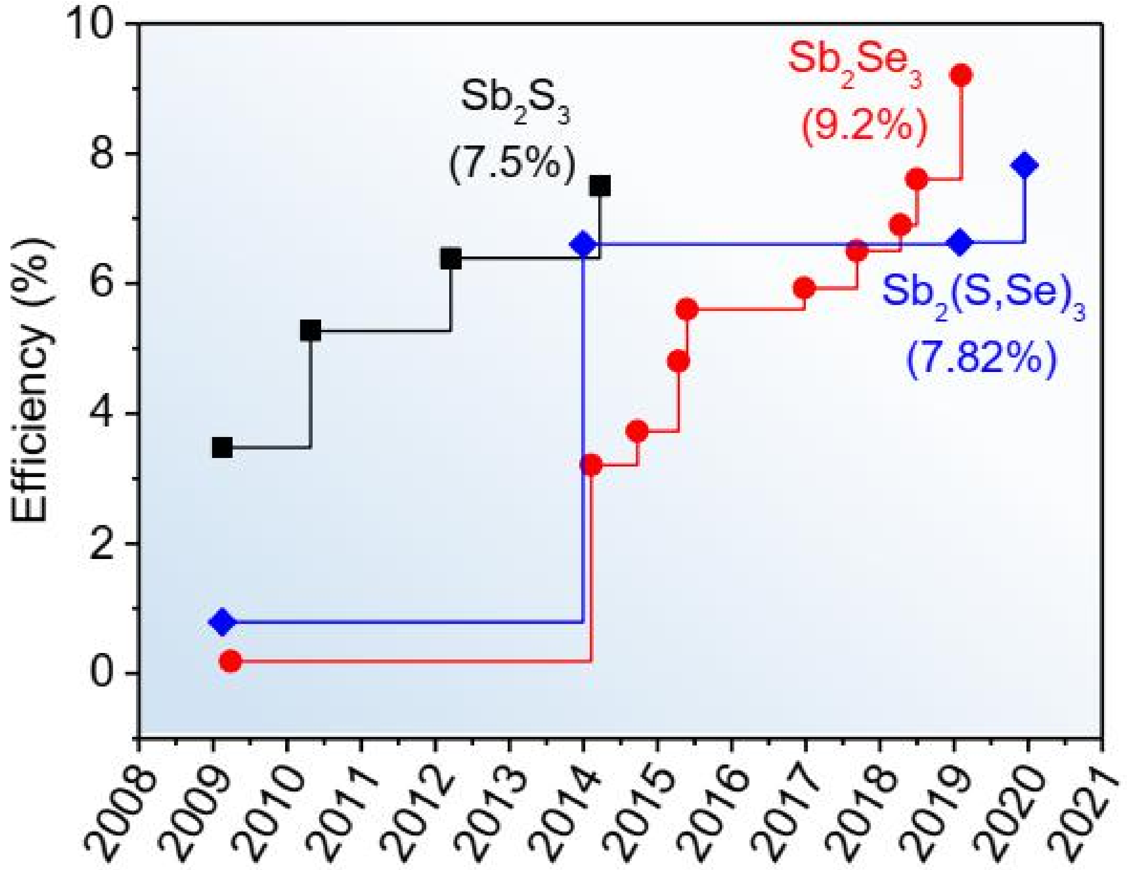
- Environmental-friendly
- Earth-abundant
- Low-cost

Easy for fabrication

- Low melting point (~615 °C)
- Binary compound (one phase)
- Stable in air

Potential in photovoltaic

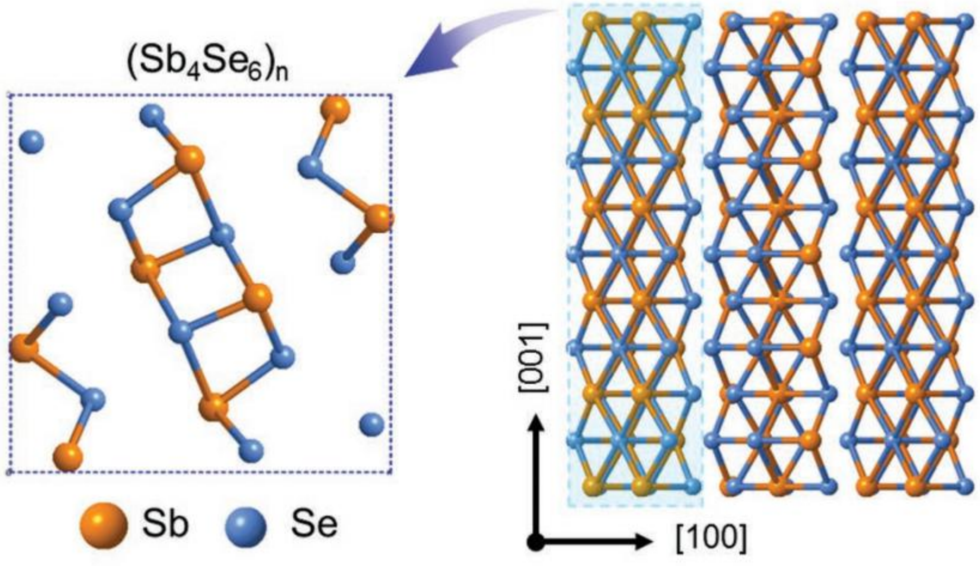
- Bandgap of ~1.1 eV
- Absorption coeffcient >10^5 cm^{-1}



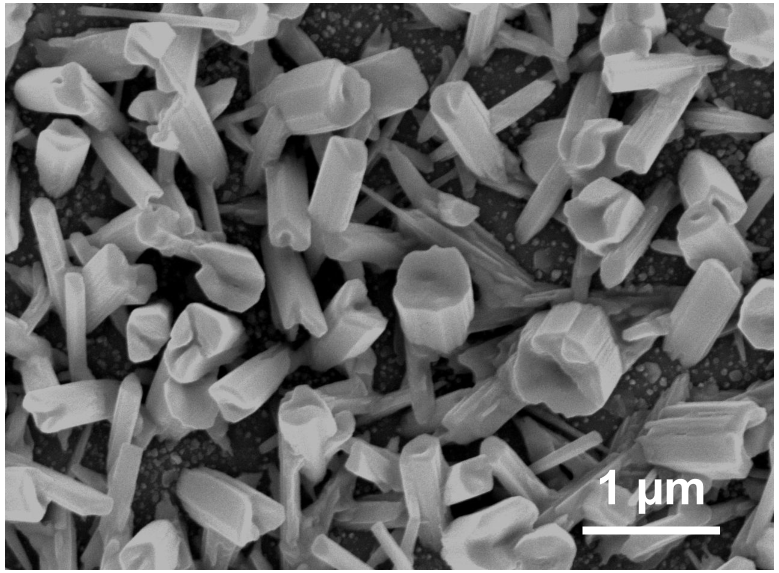
Rapid increase of PCE

C.Chen, et al. ACS Energy Letters. (accepted)

The key challenge in Sb_2Se_3 film growth



Unique 1D structure



Rod-like Sb_2Se_3 film

Ideal orientation

[hk0]: parallel to substrate

[hk1]: incline to substrate ✓

Compact film with large grain size

Sb-Se Bonding Energy > Van der Waal`s Force

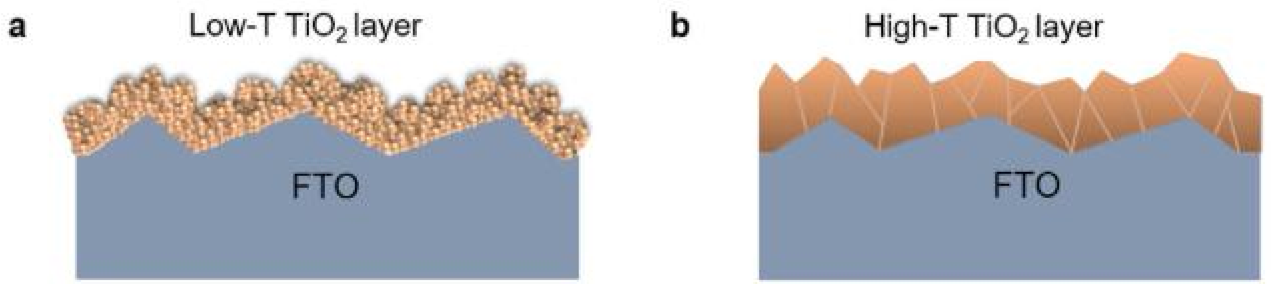
Perfer to grow along the chains (c-axis)

Our two strategies

More inert substrate

TiO_2 layer annealed at 550 °C

- Reduce the nucleation density



leadind to over 10 μm grain size Sb_2S_3 film

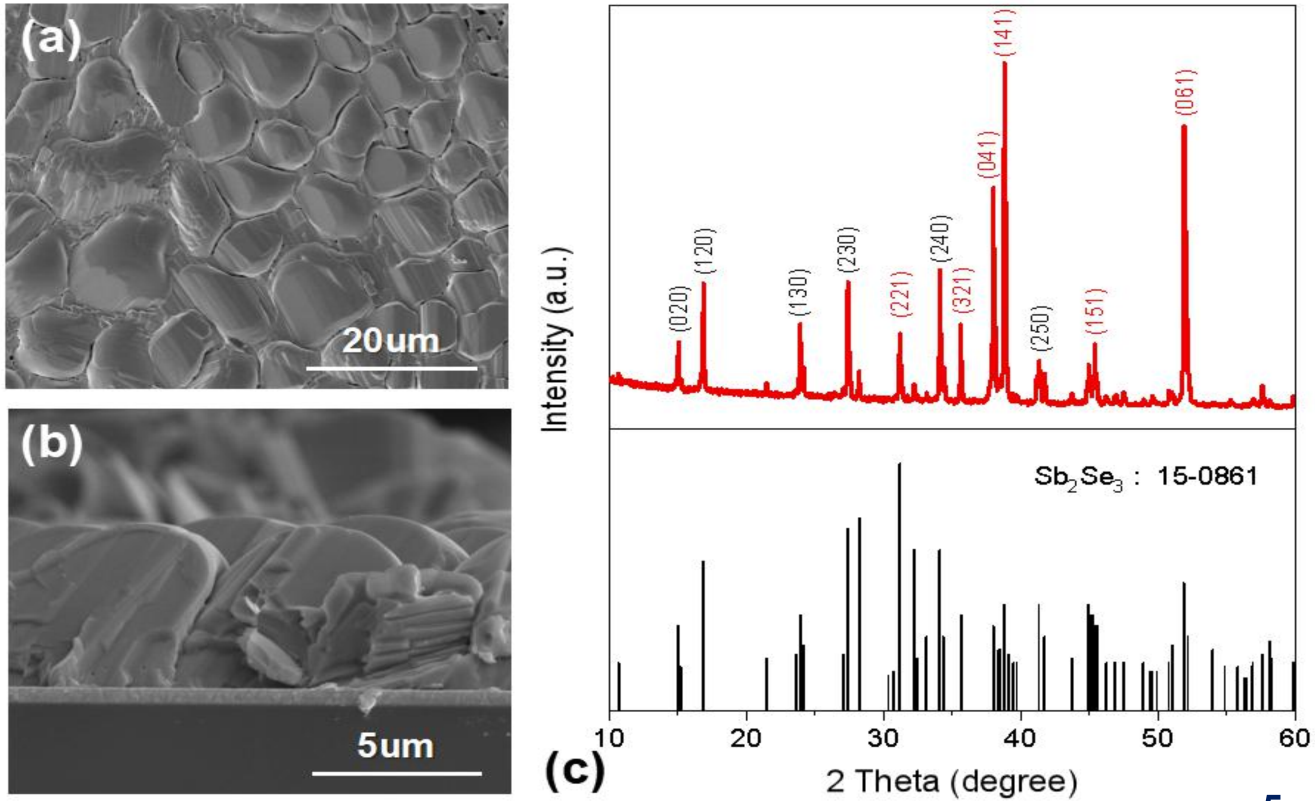
Close-spaced Sublimation

High substrate temp (400 °C)

- Bonding with substrate
- Promote [hk1] orientation

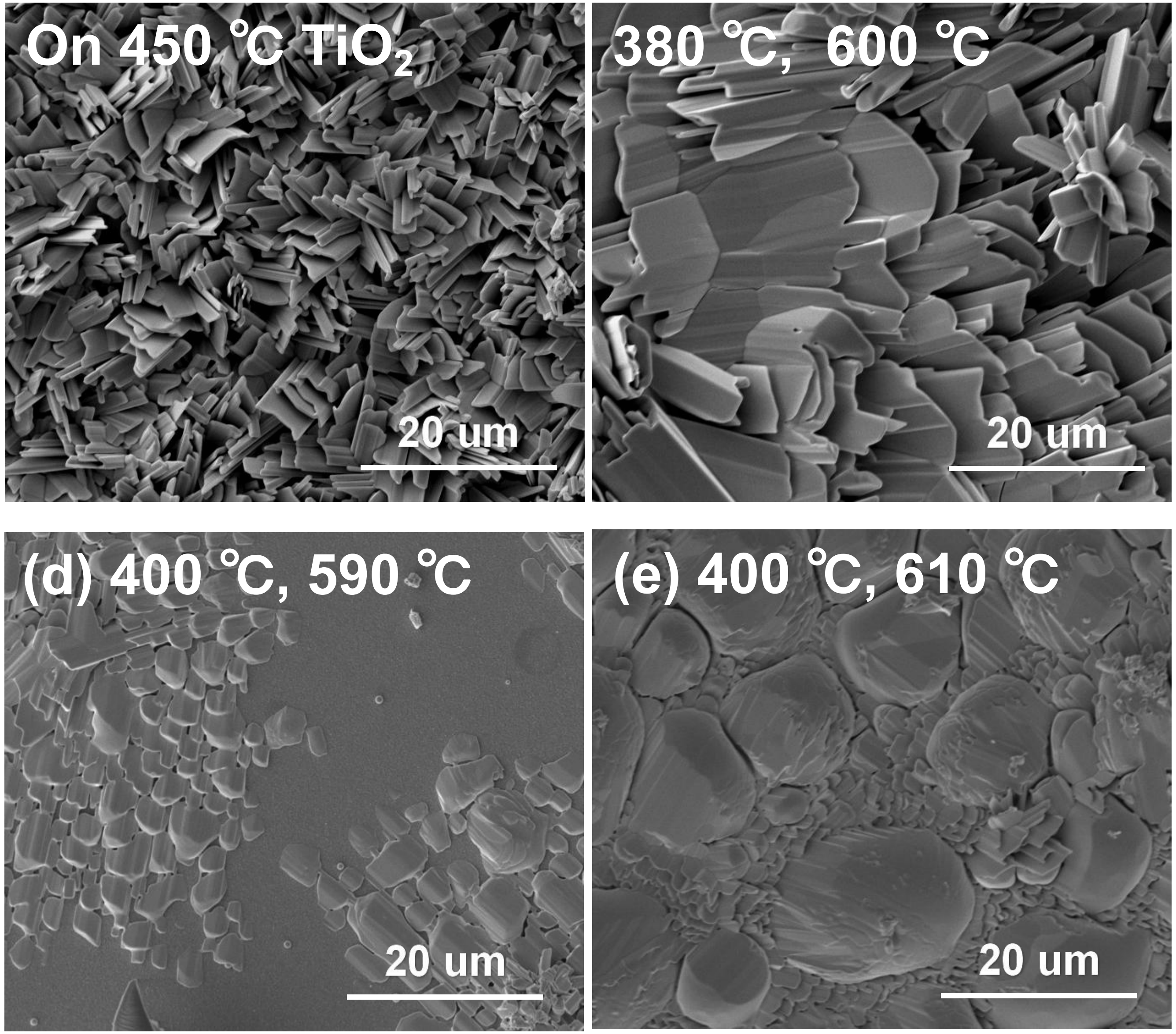
High source temp (600 °C)

- Sufficient deposition rate
- Enhance grain size



H.Deng, et al. Adv Funct Mater. 2019, 29(31): 1901720; R. Kondrotas, et al. Sol Energ Mat Sol C, 2019, 199: 16-23.

Failed attempts



Too many nuclei

- Active substrate
- Lower substrate temp
- Rod-like or sheet-like

Improper source temp

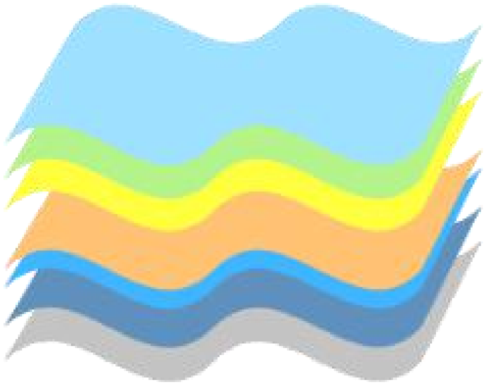
- Discontinuous film
- Small grains in gap

Summary

- Over 10 µm grain size compact Sb_2Se_3 film with [hk1] dominant orientation
- Key points:
  - Inert substrate: 550 °C annealled TiO_2 layer -> proper nucleation density
  - High substrate temp：400 °C -> bonding with substrate
  - Appropriate source temp：600 °C -> sufficient deposition rate
- However the PCE is low, possiblly due to Se deficiency under high T_{sub}

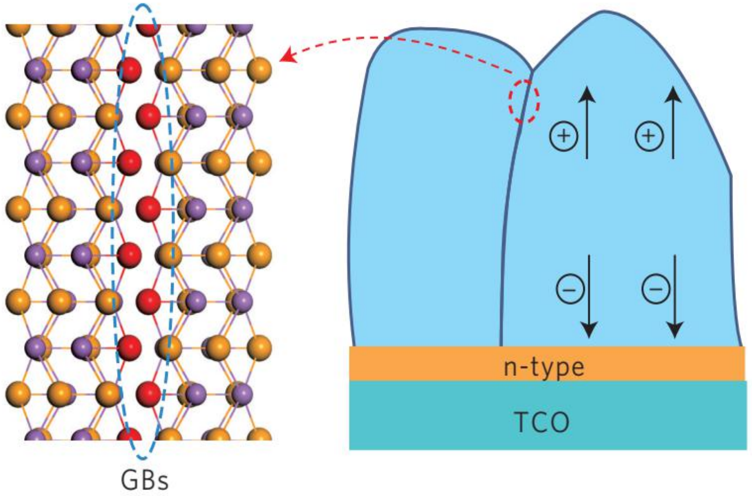
400C, 600C	Voc (V)	Jsc (mA/cm^{-2})	FF (%)	Eff (%)
Highest	0.315	15.9	43.1	2.16
V.A.	0.324	12.3	43.4	1.73
SD/VA.	0.045	0.184	0.018	0.202

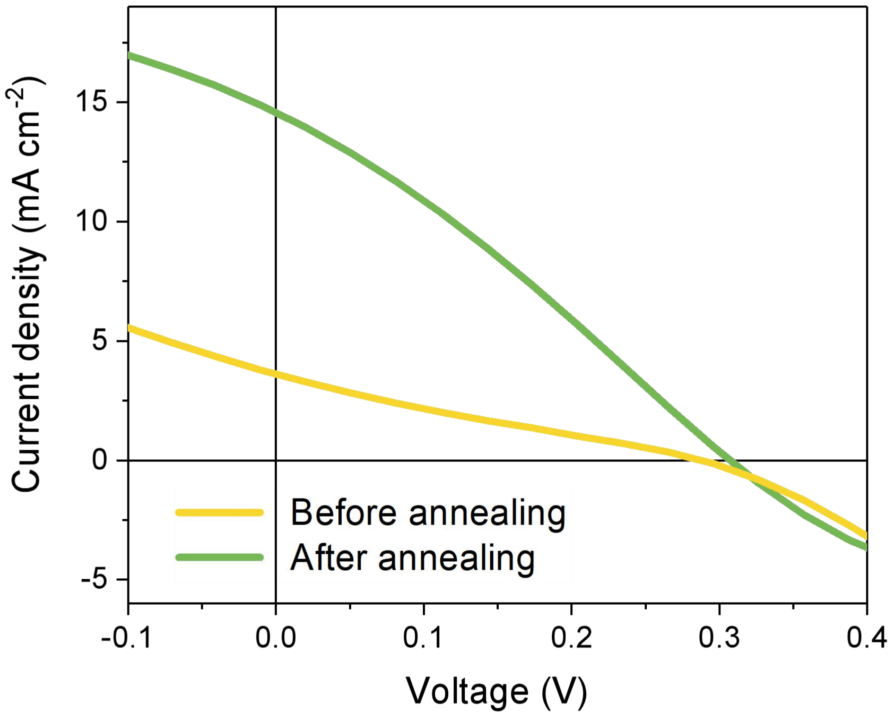
The importance of surface passivation



$NH_3 \cdot H_2O$
25% wt

Sb_2Se_3 is disoluble in $NH_3 \cdot H_2O$



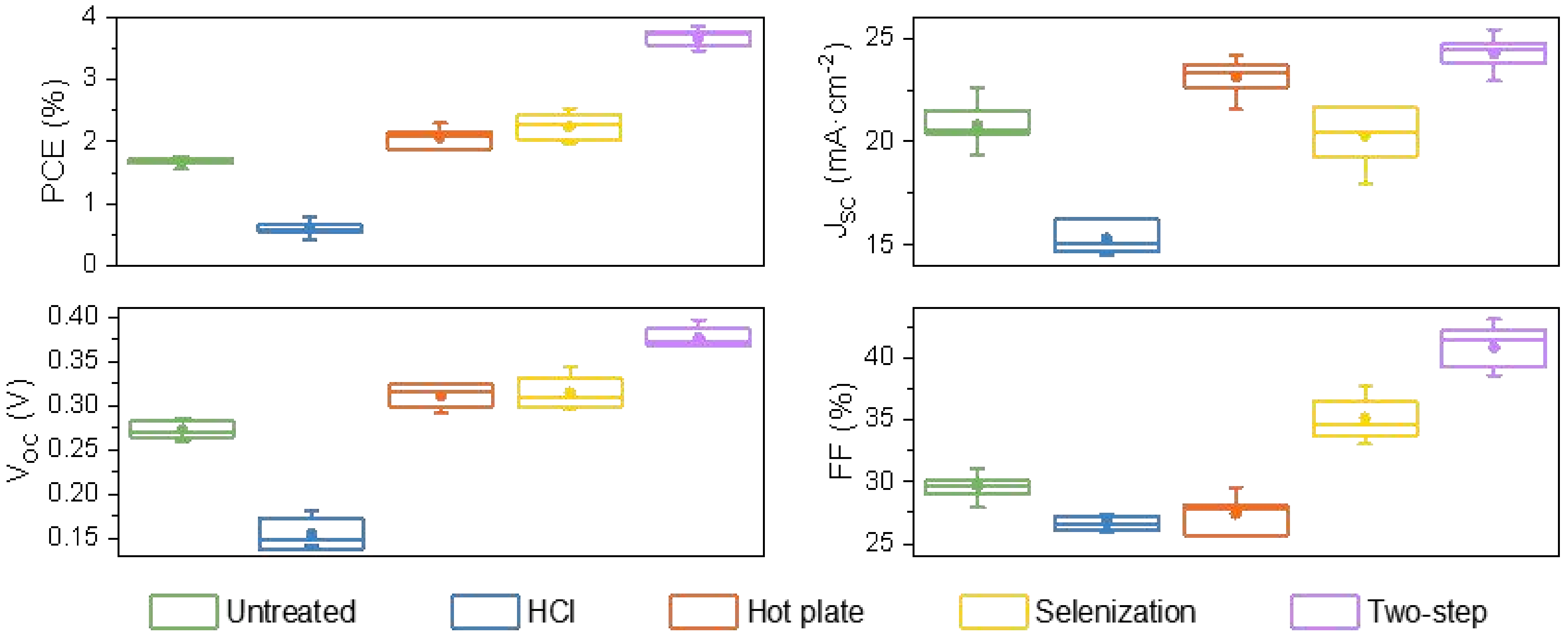


Extremely important in substrate structure

- CBD process damage Sb_2Se_3 surface
- Lots of dangling bonds on surface
- Surface defects block photo current

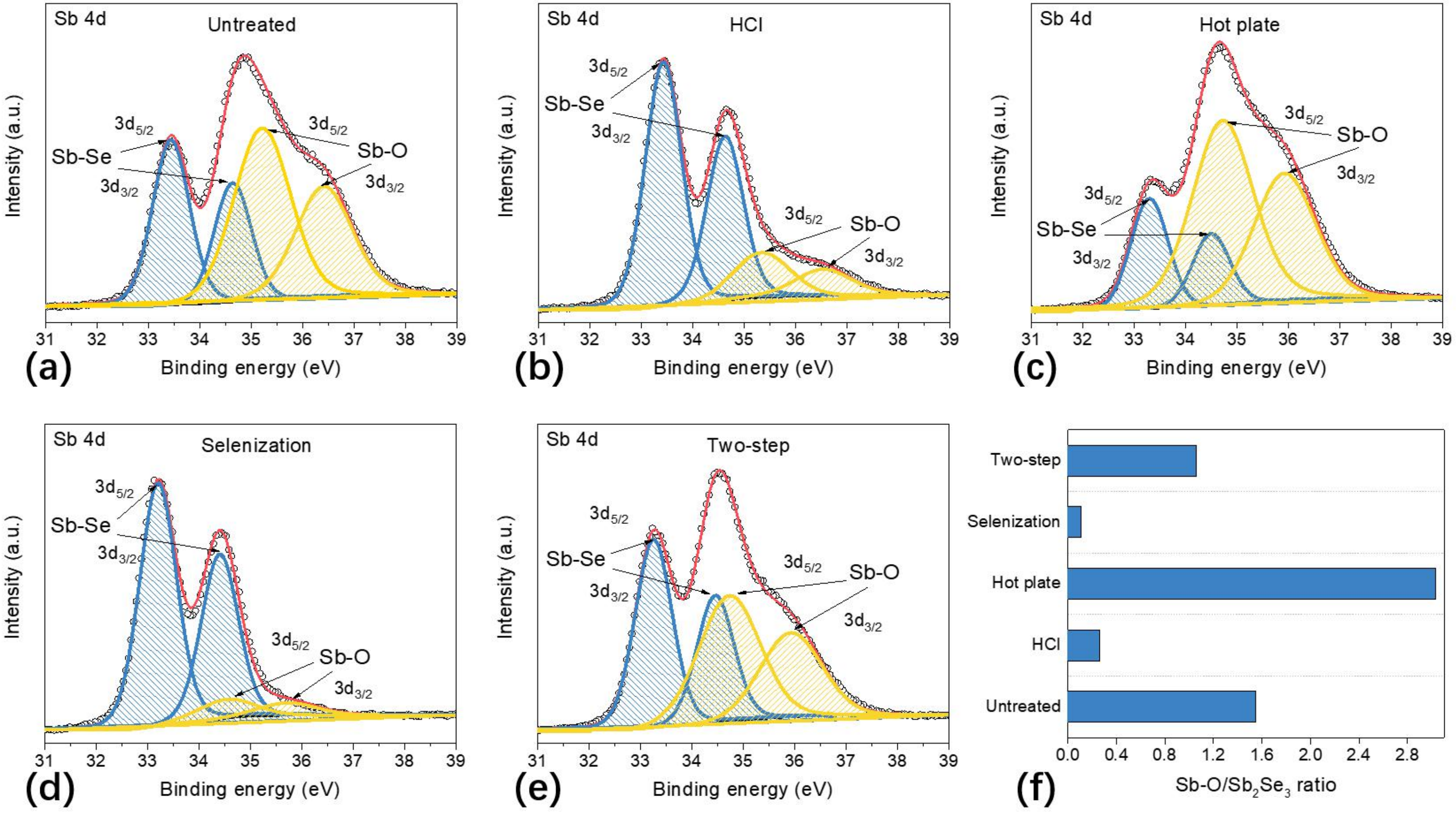
Y.Zhou, et al. Nat Photonics, 2015, 9(6): 409-415.

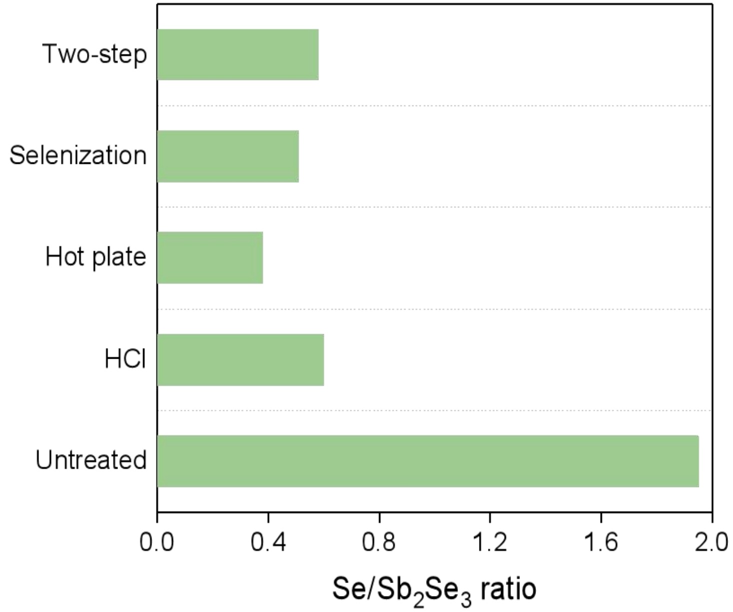
Four surface treatment attempts



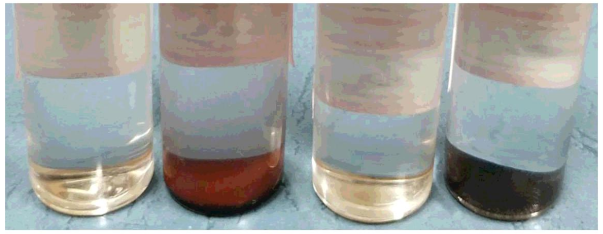
- Thermal evaporated In_2S_3 buffer layer was developed to avoid surface damage
- Two-step method is the best (HCl etching 30s; Hot plate 300 °C 60s in air)

XPS analysing





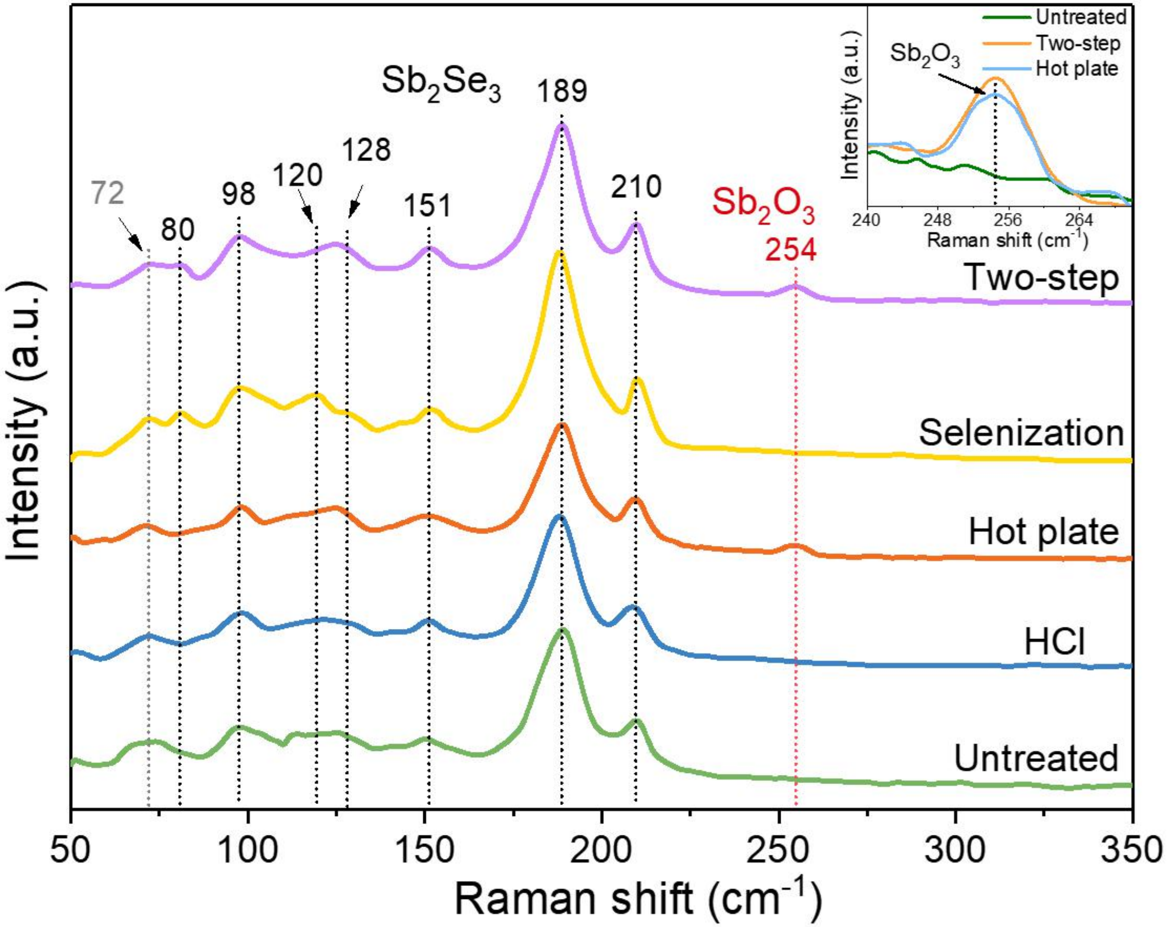
HCl
36% wt

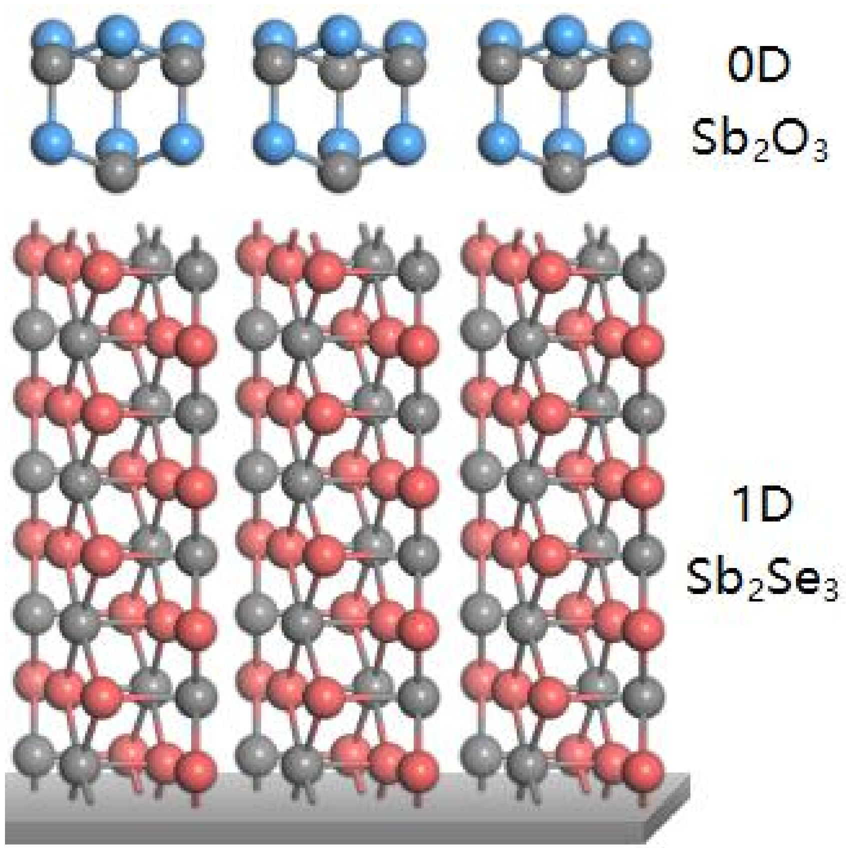


Sb_2O_3 and Sb_2Se_3 are disoluble in HCl

- After treatment, Sb-O compound has significant difference
- Se compound is almost same between various method

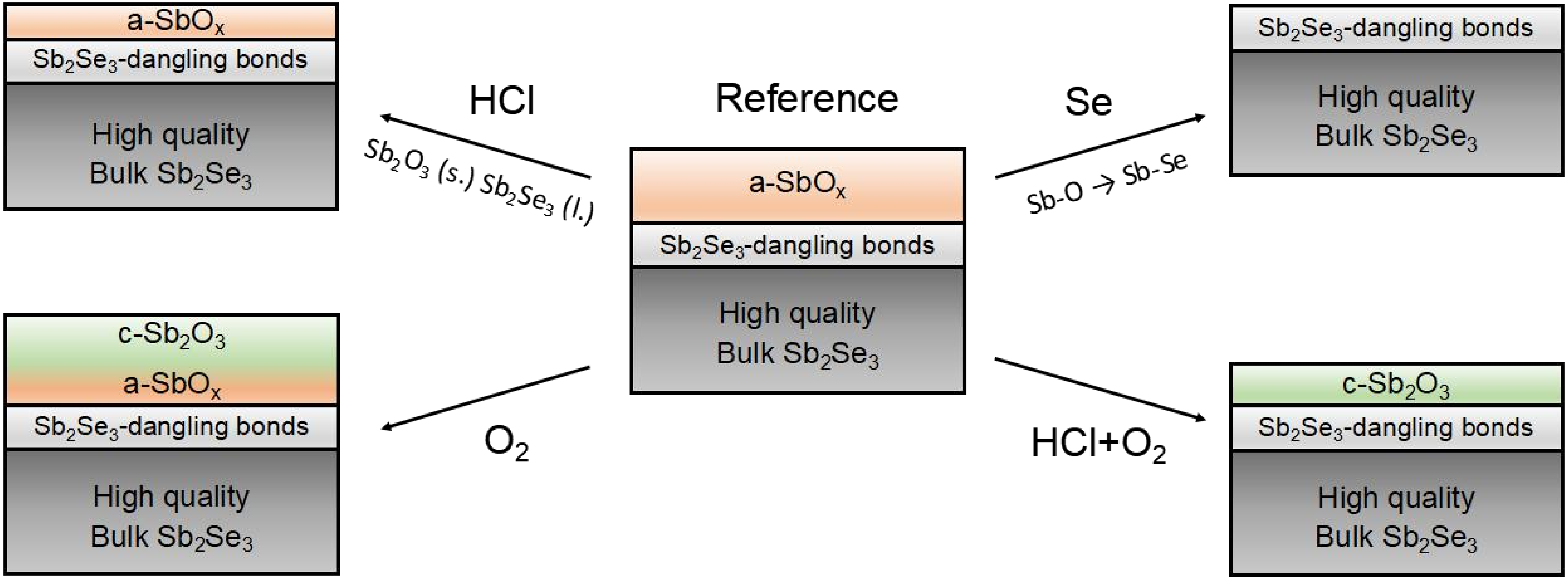
Raman spectrum and crystal structure





- Only high temperature annealed sample has Sb_2O_3 peak at 254 cm^{-1}
- Sb_2O_3 is 0D structure material without any dangling bonds

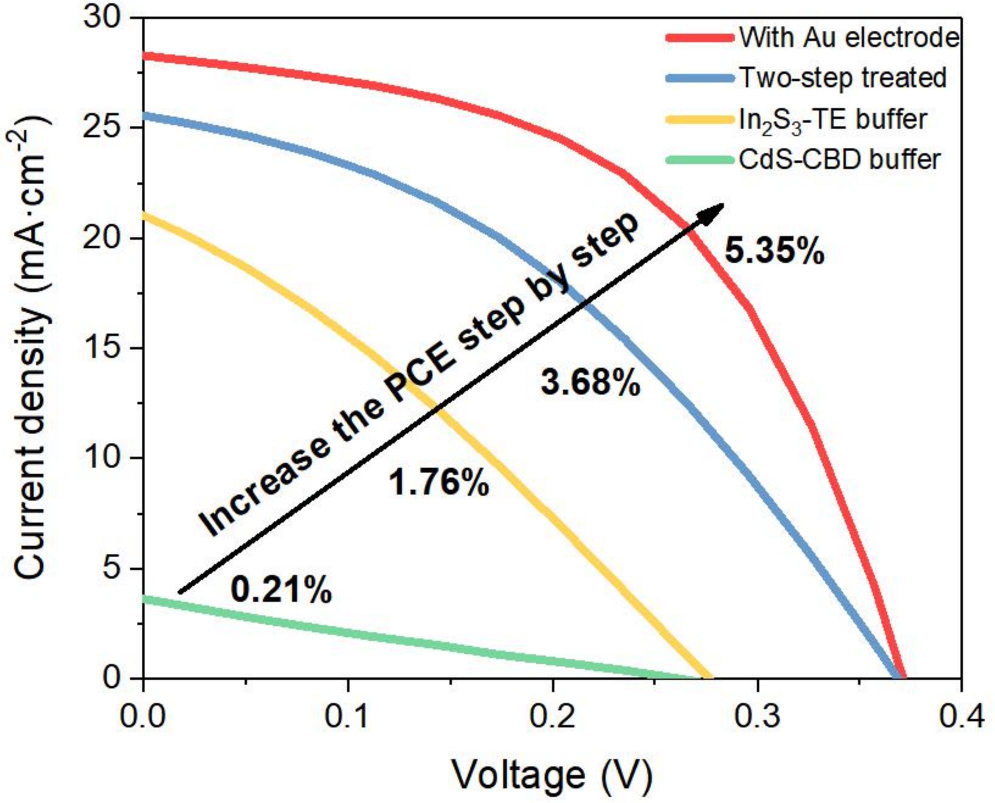
Passivation model

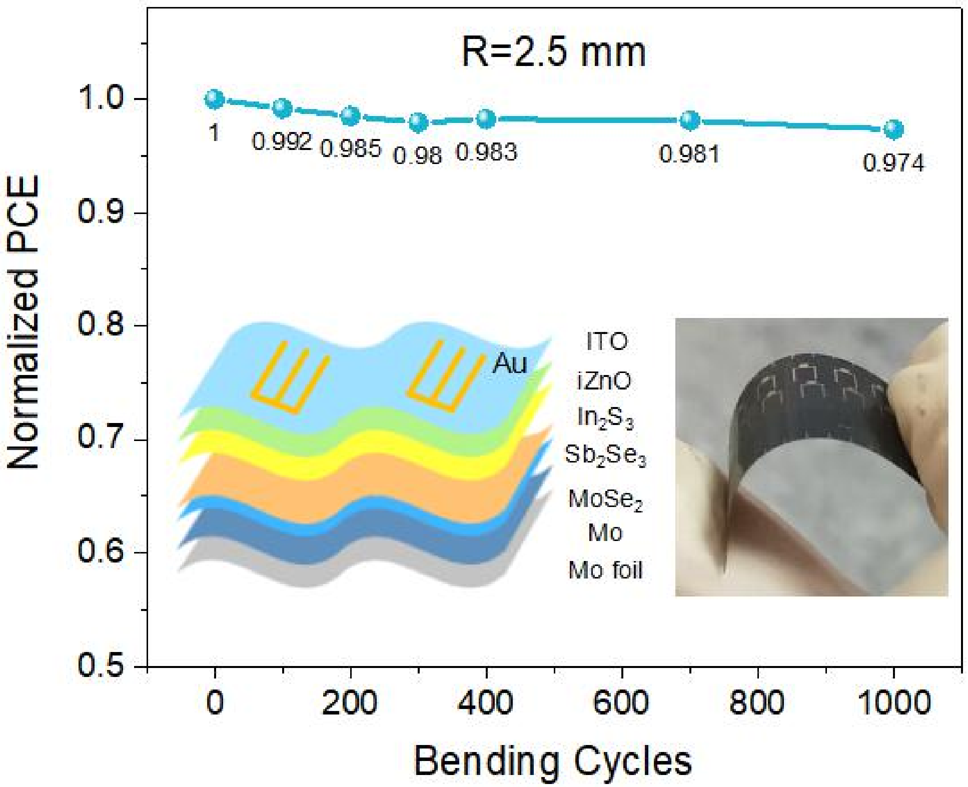


- Firstly, remove contaminative layer (a-Sb_2O_3) by HCl etching
- Secondly, form a high quality 0D c-Sb_2O_3 passivation layer on hot plate

Summary

- Thermal evaporated In_2S_3 non-toxic buffer layer was explored
- Simple two-step surface passivation method was developed
- 5.35% PCE flexible Sb_2Se_3 solar cell was fabricated





C.Wang, et al. Nano Energy, 2020, 71: 104577.

Acknowledgements

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Thanks for your attention!

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