

Phase characteristics and optical properties of tetrahedrite $\text{Cu}_{12}\text{Sb}_4\text{S}_{13}$ and $\text{Zn}_x\text{Cu}_{12}\text{Sb}_4\text{S}_{13}$ thin films prepared by AACVD

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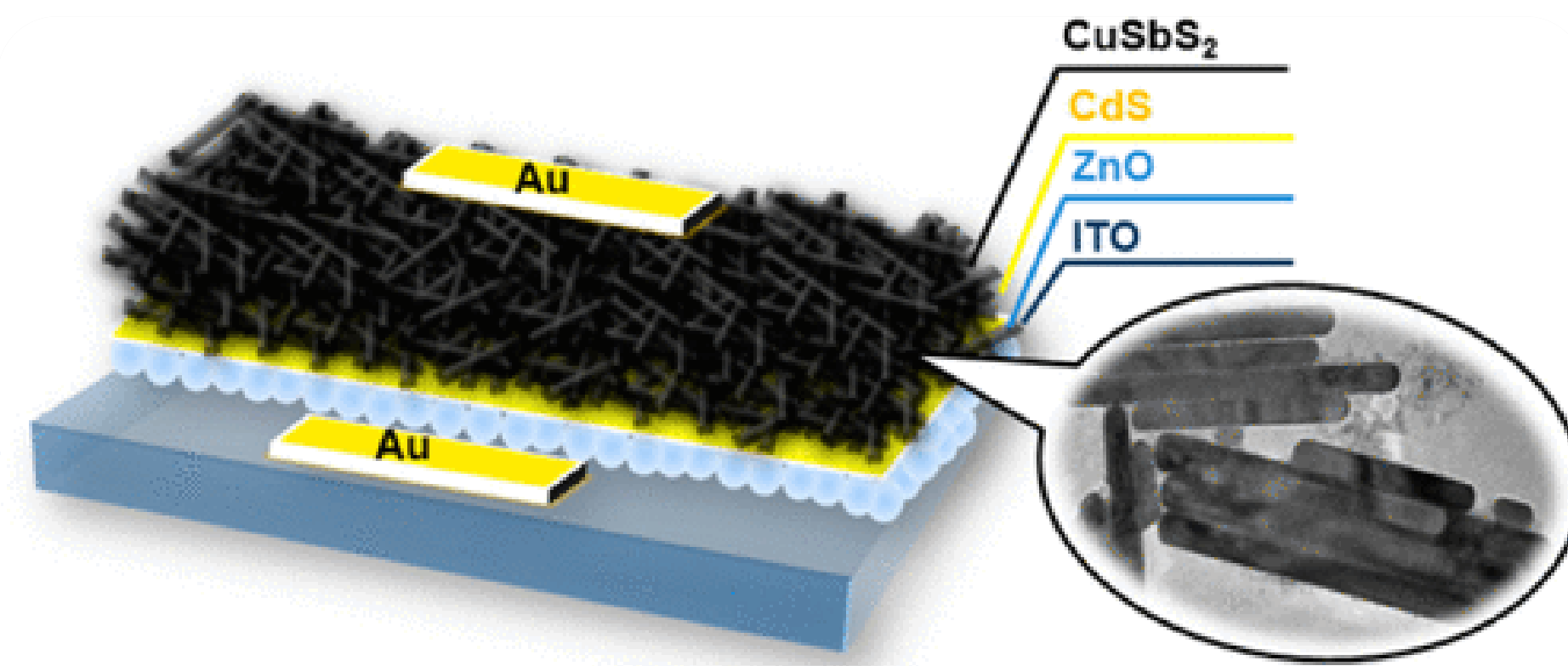


Introduction

Cu-Sb-S is a superb candidate for photovoltaics because it has:

- **Excellent, broad variation of intrinsic functional properties**
- **Structure, composition, and stoichiometry versatility**
- **Earth abundance, low cost, environmental and benign health effects**
- **Tunable bandgap**

Fig 1. Cu-Sb-S absorber in p-n junction solar cell¹



AACVD Synthesis

- Deposition of **equimolar quantities** of aerosolized **Cu & Sb dithiocarbamate** precursors dissolved in **20 mL THF** onto **glass substrates** was carried out at **500, 550 and 600 °C** for **1 hour** @ **130 and 150 sccm**.

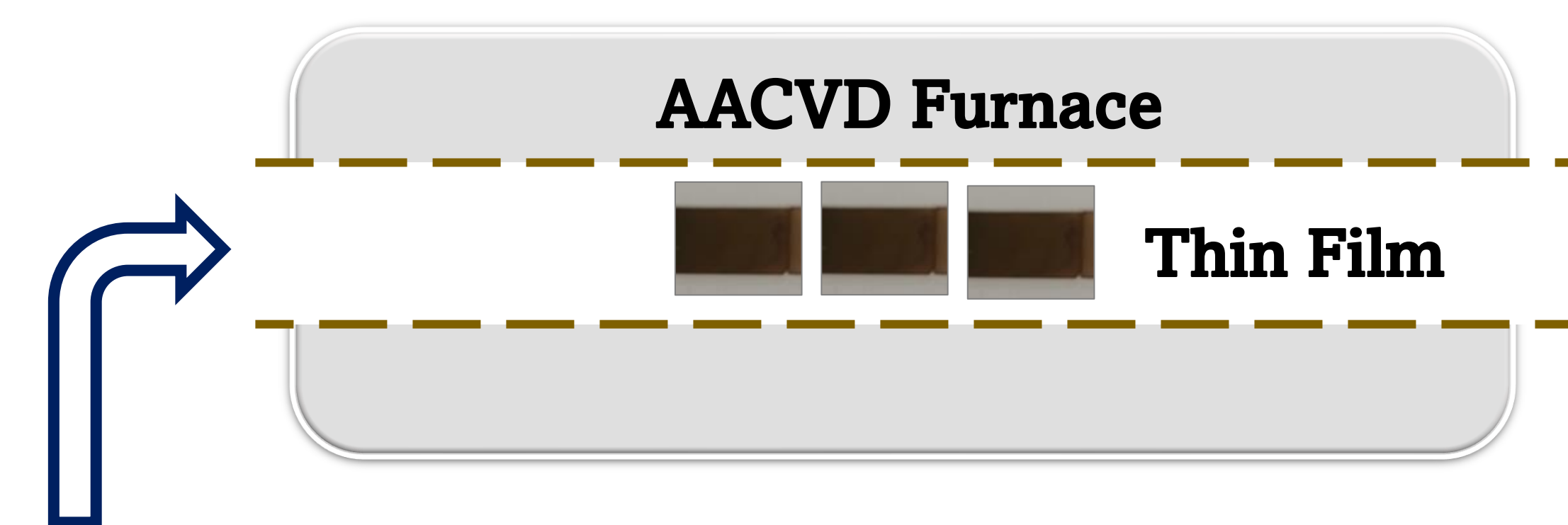


Fig 2. Diagram of AACVD set up

Structural Characterization

- pXRD, XPS & Raman data confirm **cubic structure** despite reaction conditions.
- SEM-EDS suggest a correlation of **composition** of tetrahedrite phase $\text{Cu}_{12}\text{Sb}_4\text{S}_{13}$ with **particle sizes** ranging from 0.1 to 4 μm .

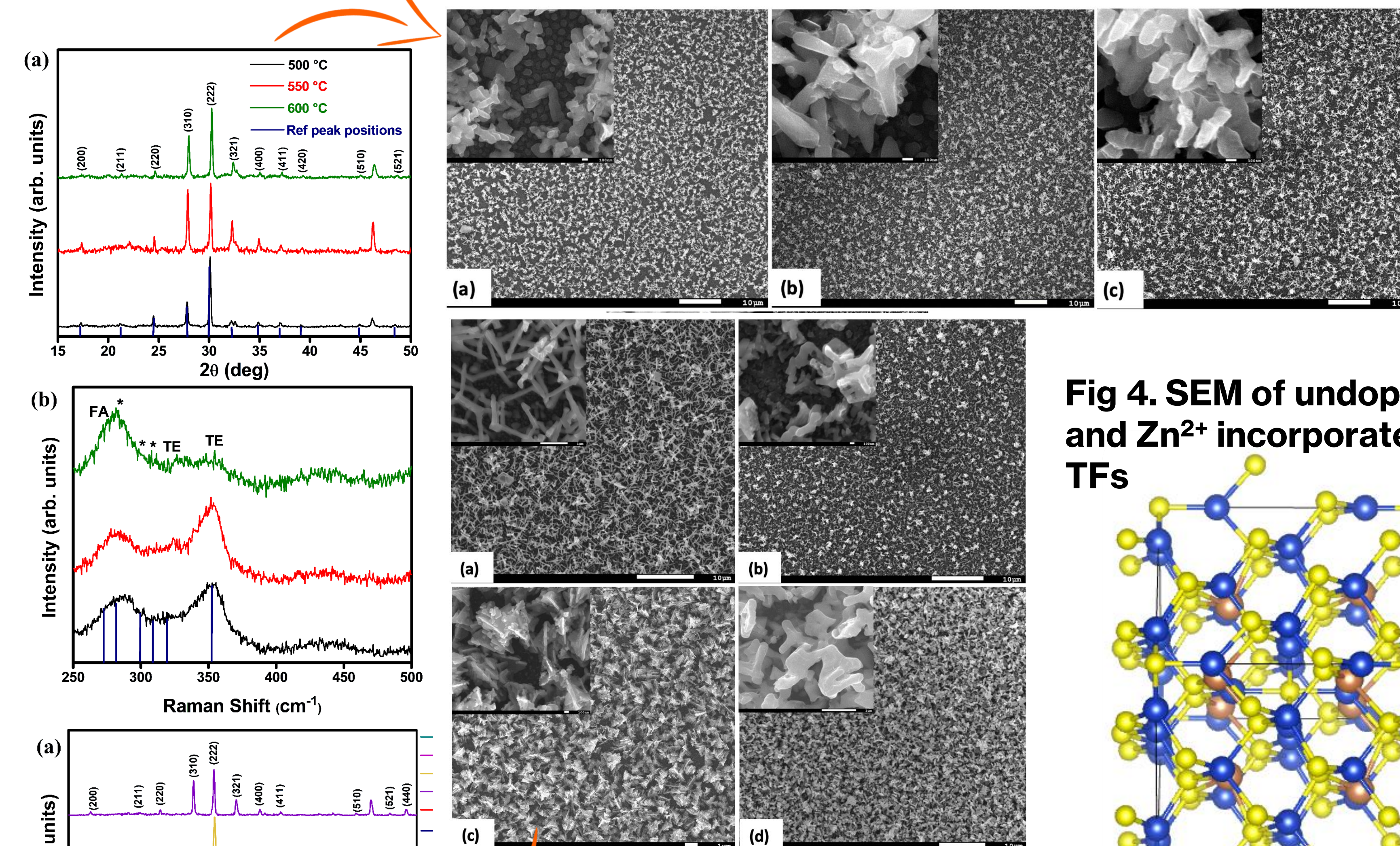


Fig 4. SEM of undoped and Zn^{2+} incorporated TFs

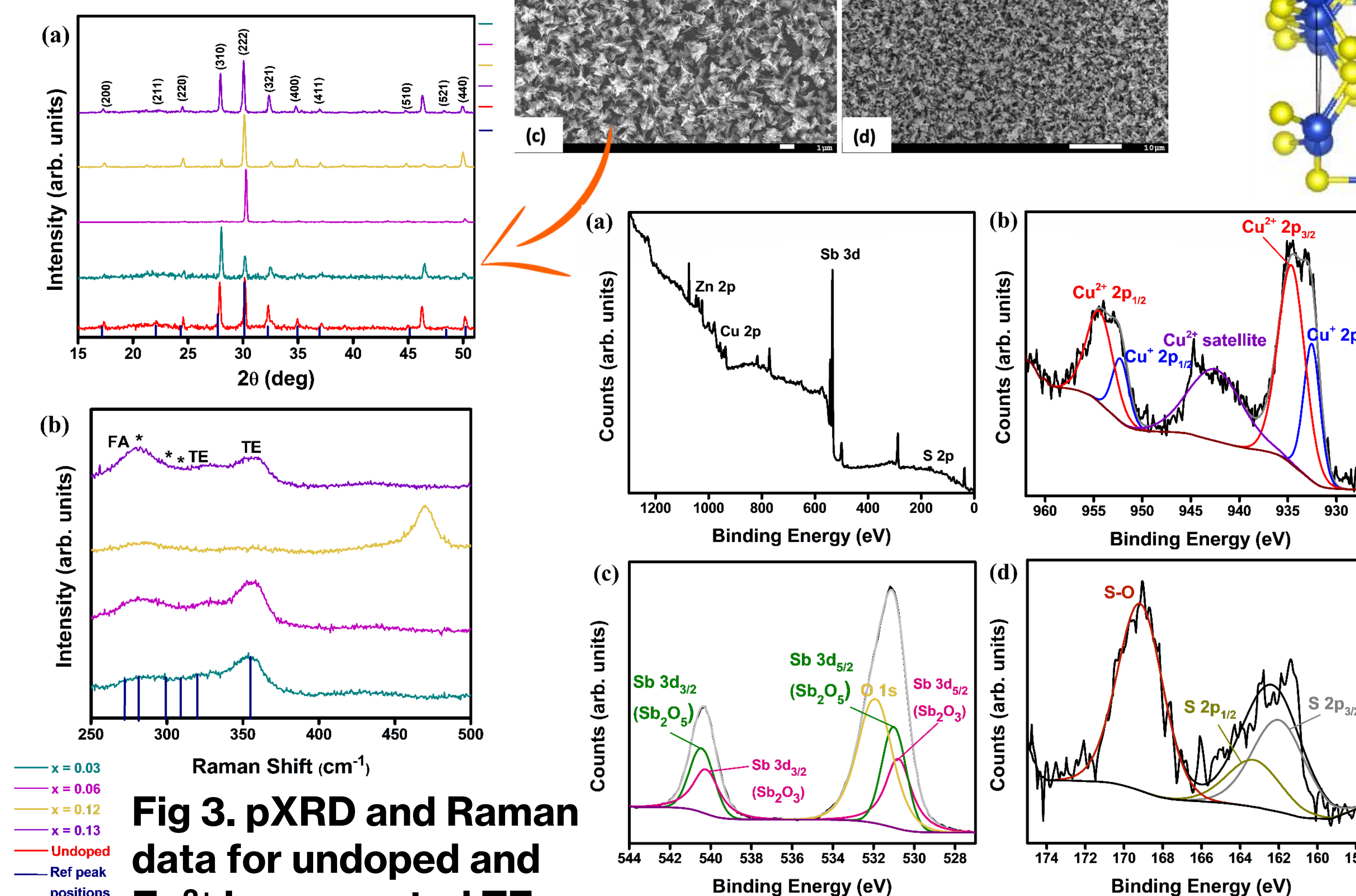


Fig 5. Representative XPS spectra of undoped CAS TFs

Optical Properties

- Undoped TFs absorb in the **visible** region with **indirect band gap** of **~2.1 eV**.
- Zn^{2+} incorporated films are narrowed with a range between **1.7 – 1.9 eV**.

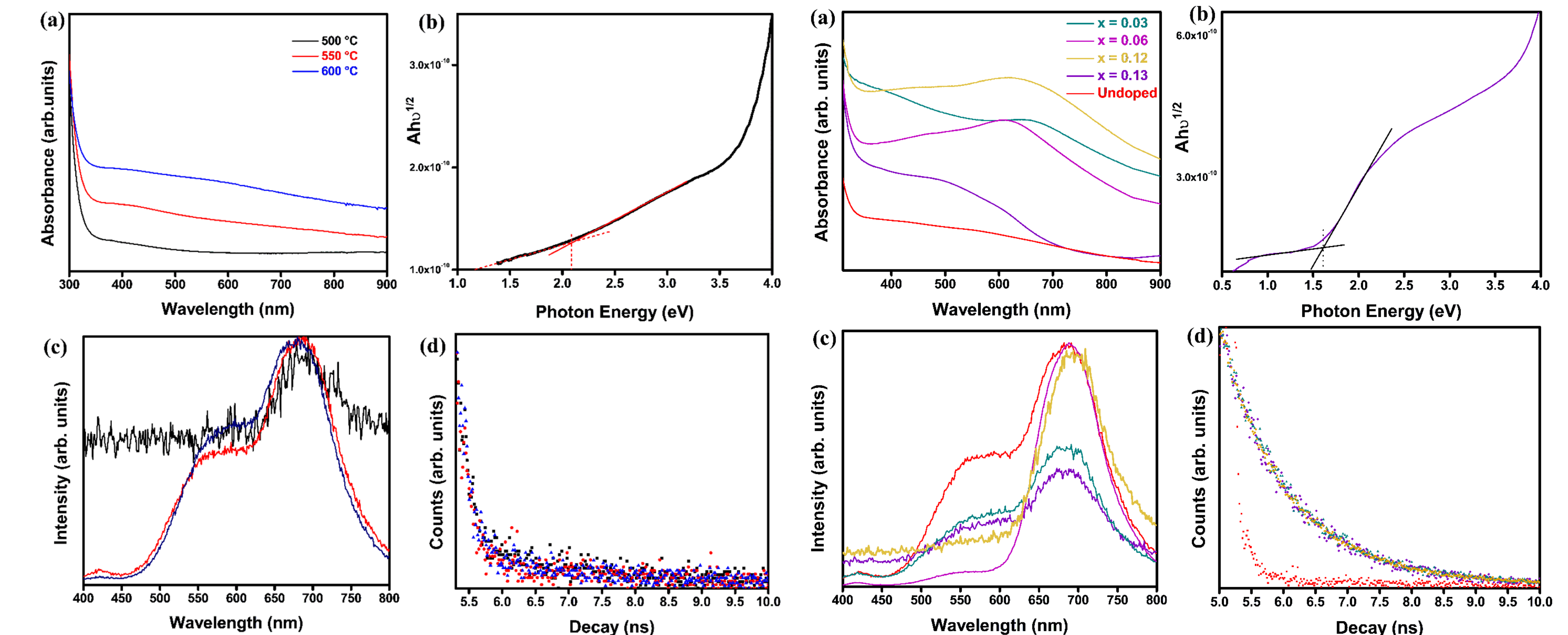


Fig 6. Optical spectra undoped and Zn^{2+} incorporated CAS TFs

Electrochemical Properties

- TFs deposited on FTO/ITO as working electrodes substrates display **reversible redox reactions** suggesting good stability.

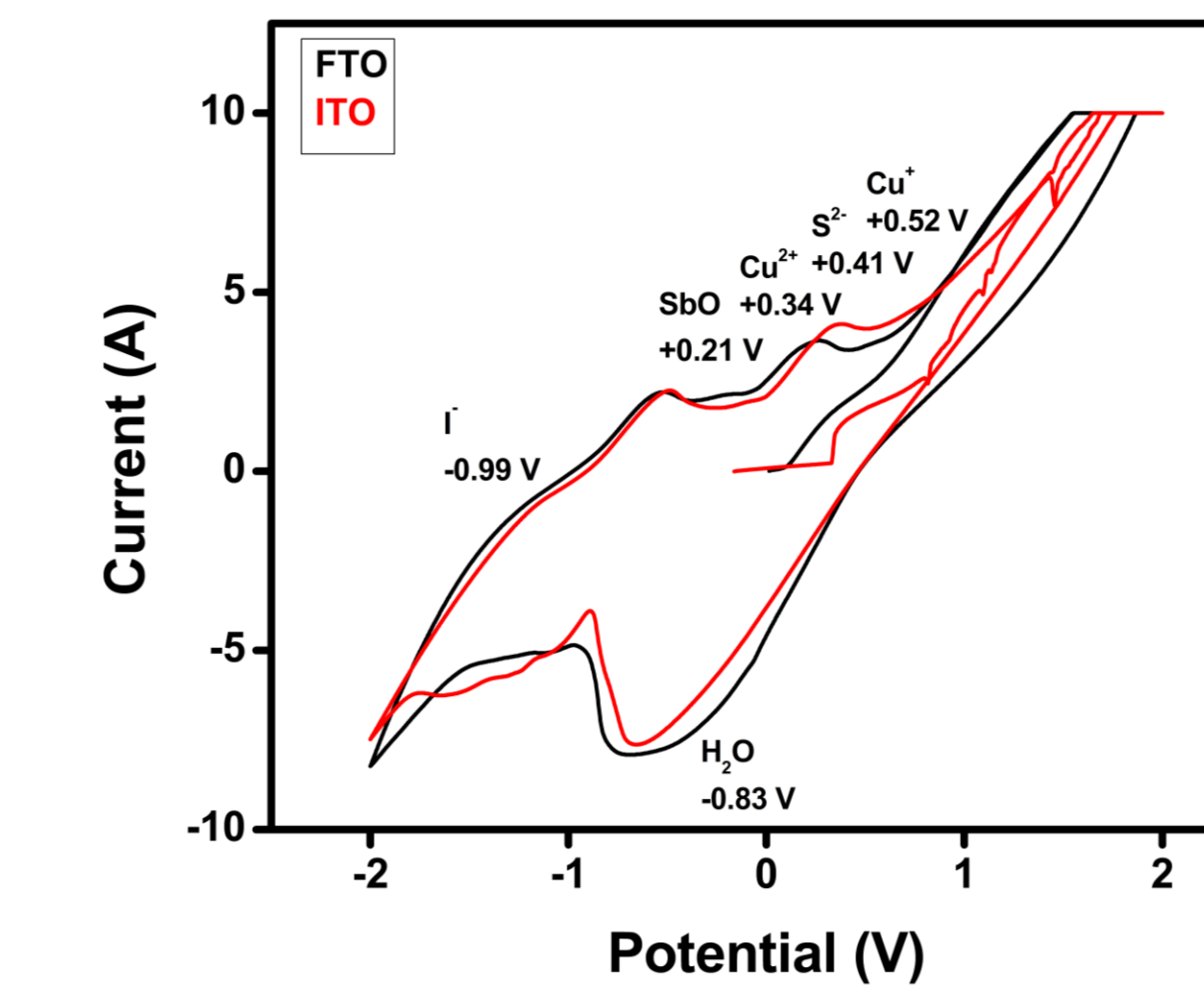


Fig 8. CV of CAS TFs deposited on FTO/ITO substrates

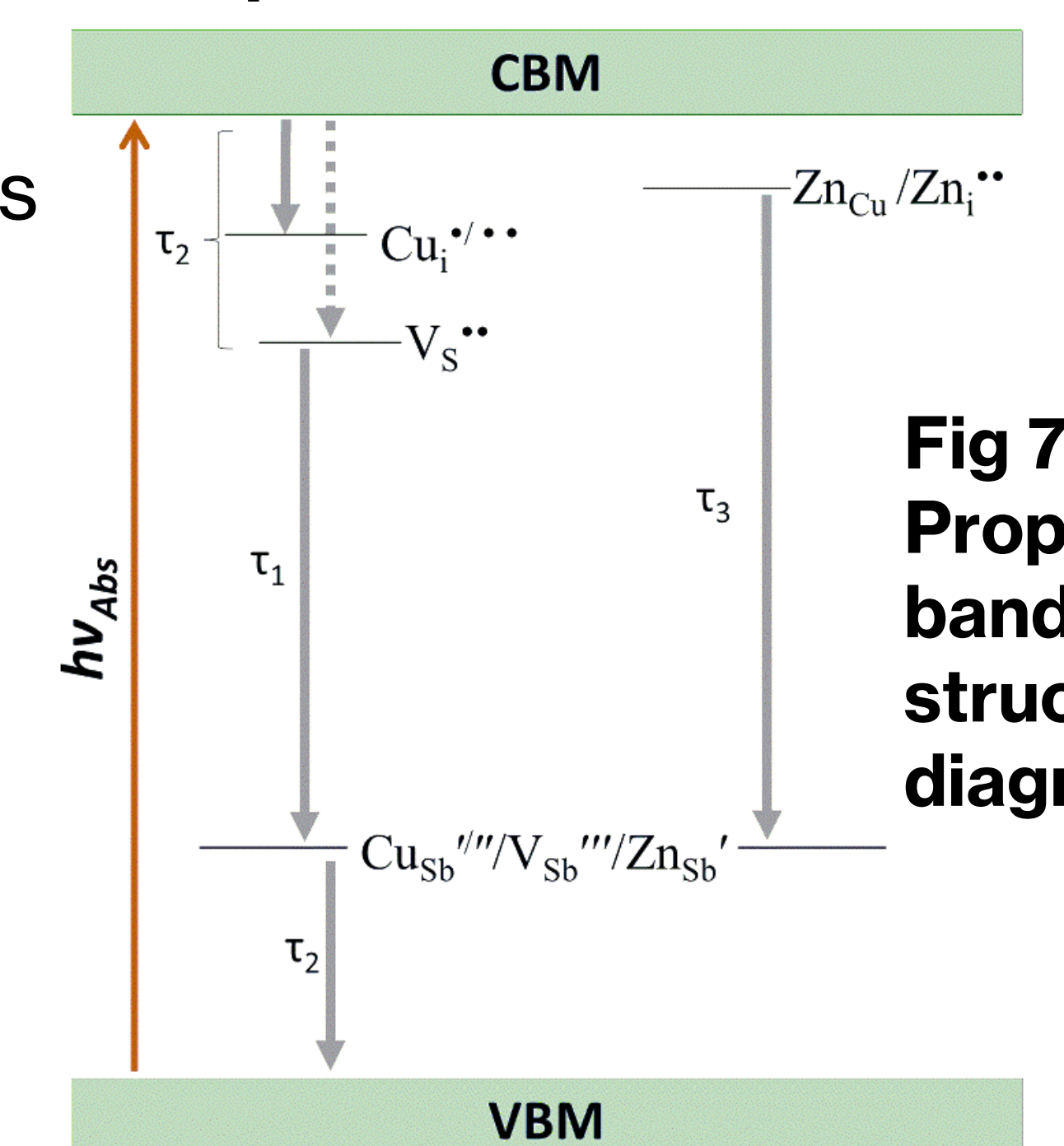


Fig 7. Proposed band structure diagram

Conclusions

- AACVD produced tetrahedrite $\text{Cu}_{12}\text{Sb}_4\text{S}_{13}$ thin films at variable temperature and flow rates to control morphology, composition, optical and electrochemical properties for photovoltaics and catalysis.

References

1. Suehiro, S.; et. al; *Inorganic Chemistry* 2015, 54 (16), 7840-7845.

