Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Exploring the Application of Quaternary Metastable Wurtzite Nanocrystals in Pure-sulfide Cu_2ZnSnS_4 Solar Cells by Forming Nearly Micron-sized Large Grains

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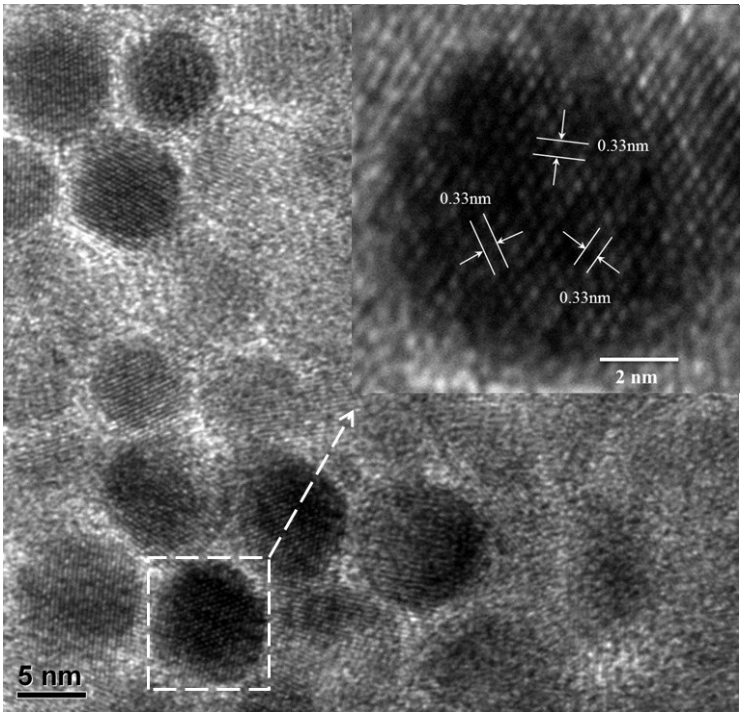

Figure SI 1. TEM image of as-prepared wurtzite CZTS nanocrystals. The inset shows the corresponding high resolution TEM image

The lattice fringes with an interplanar spacing of 0.33 nm are ascribed to the {100} planes of wurtzite CZTS [1].

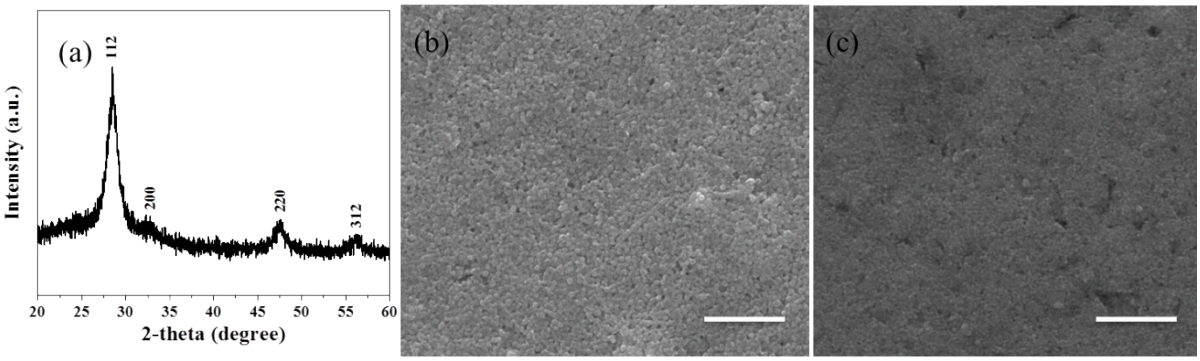

Figure SI 2. (a) XRD patterns of as-prepared CZTS films made from kesterite nanocrystals before sulfurization; (b) Top-view SEM image of as-deposited CZTS films made from kesterite CZTS nanocrystals before sulfurization; (c) Top-view SEM image of as-deposited CZTS films made from kesterite nanocrystals after sulfurization. (Scale bar is 2μm)

In comparison with the films made from wurtzite CZTS nanocrystals, the morphology of the films made from kesterite CZTS nanocrystals kept identical under the same sulfurization condition. No clear growth of grains was observed.

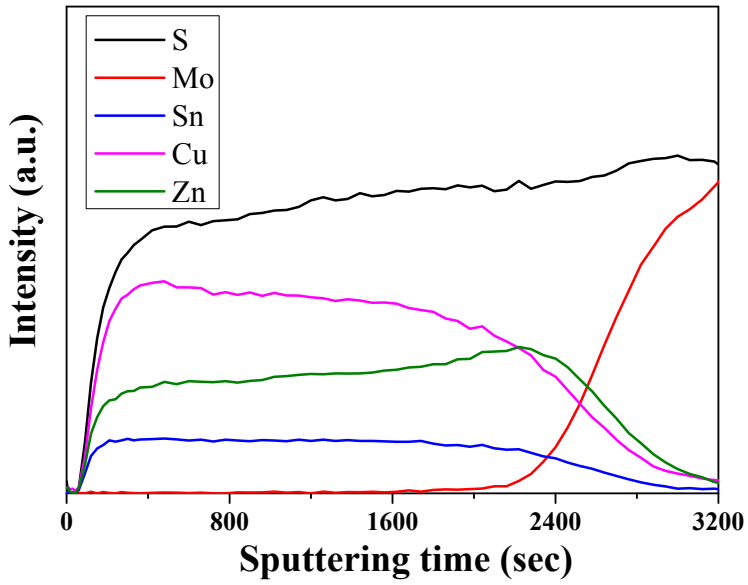

Figure SI 3. Composition depth profile taken along the sulfurized CZTS absorber layer.

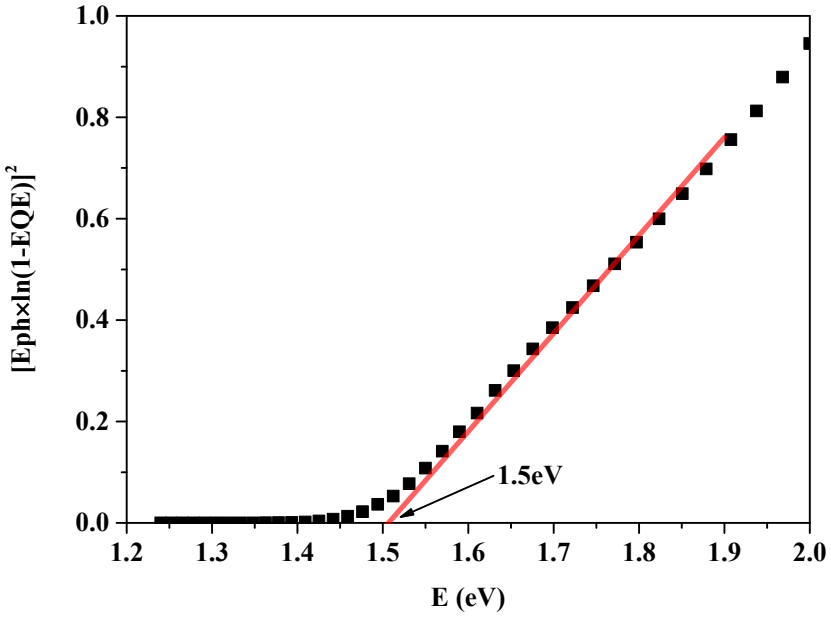

Figure SI 4. The band gap were estimated to be approximately 1.5 eV from the plot of [E * ln(1-EQE)]2 vs. E, where E is the photon energy.

According to the equation of literature[2], the band gap of the final CZTS absorber estimated from EQE data is about 1.5 eV.

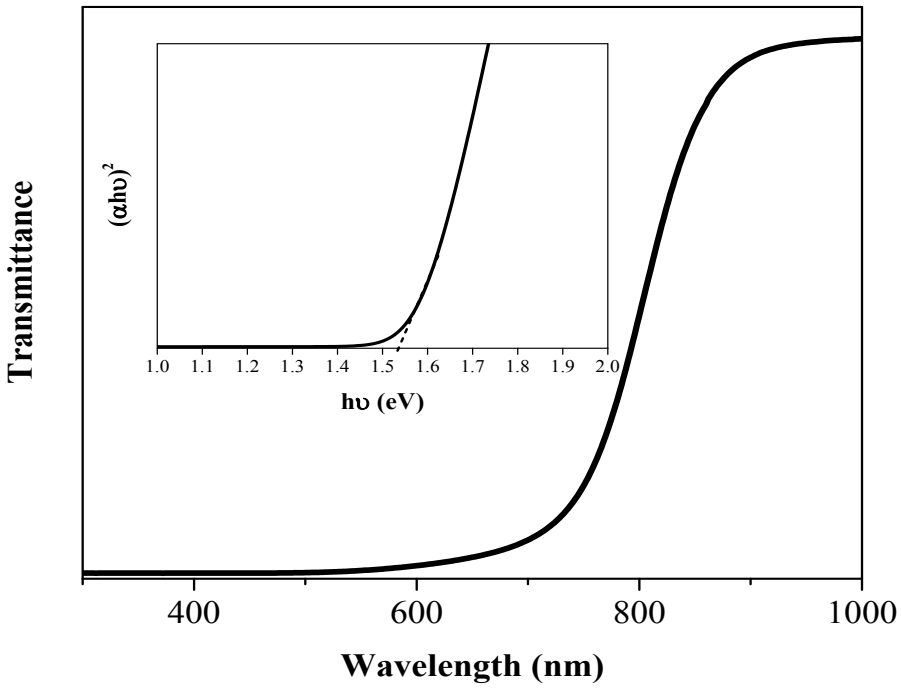

Figure SI 5. Transmittance spectra of the final CZTS absorber. Inset is a plot of (αhv)2 vs hv for the absorption spectra.

The band gap of the final CZTS absorber estimated from the transmission spectra is about 1.52 eV, which is very close to the 1.5eV estimated from EQE data.

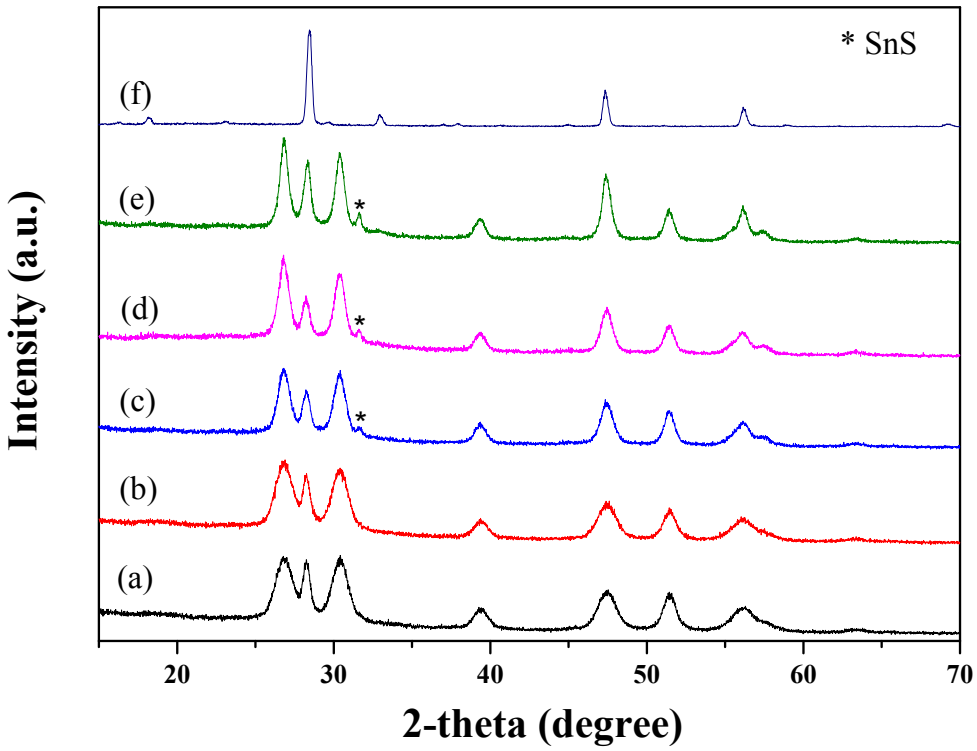

Figure SI 6. XRD patterns of (a) as-deposited CZTS precursor films before sulfurization, (b-e) The CZTS thin films were taken out from the furnace at different temperatures and the temperatures were (b) 350°C，(c) 400°C, (d) 450°C, and (e) 500°C, and (f) the final CZTS absorber annealed at 580°C for 5 min. SnS (*) was detected during the heating process.

The detection of SnS peak confirms that the Cu/Sn ratio in CZTS is self-regulated and excess Sn evaporates in the form of SnS if precursor films are initially Sn rich.

References

[1] X. Lu, Z. Zhuang, Q. Peng, and Y. Li, Chem. Commun., 2011, 47, 3141.

[2] J. Ge, J. Jiang, P. Yang, C. Peng, Z. Huang, S. Zuo, L. Yang, and J. Chu, Solar Energy Materials & Solar Cells, 2014, 125, 20.