

Growth mechanism of CZTSSe absorber layers during selenization of stack precursor

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The family of kesterite compounds, including $\text{Cu}_2\text{ZnSnS}_4$ (CZTS), $\text{Cu}_2\text{ZnSnSe}_4$ (CZTSe) and the sulfo-selenide $\text{Cu}_2\text{ZnSn}(\text{S},\text{Se})_4$ (CZTSSe), draws increased attention for the production of low cost thin film solar cells since they mainly consist of earth abundant or readily available elements. Kesterite can be derived from the well-known chalcopyrite absorber material $\text{Cu}(\text{In},\text{Ga})\text{Se}_2$ by substituting In and Ga (both group III elements) by Zn (group II) and Sn (group IV) atoms.

The current record efficiency for copper zinc tin sulfide–selenide (CZTSeS) thin film solar cells using a solution technique is 12.6% , while CZTS solar cells fabricated using vacuum techniques approach an efficiency of 9.3%. [1~3] Almost all of the aforementioned deposition techniques involve two steps. First, metal containing precursors with or without chalcogen addition are deposited, and second, the precursors are annealed under optimized conditions in a sulfur/selenium containing atmosphere to yield the final kesterite phase. In this respect, the knowledge of the formation and conversion reactions that occur during the annealing step is essential for obtaining phase-pure CZTS(Se) absorbers with targeted metal ratios. This study presents a detailed insight into the phase formation processes of CZTSSe during the selenization of metal compound precursors. Several complementary characterization techniques are employed to identify intermediate phases. We also investigate the influence of annealing condition on CZTSSe film properties and solar cell performance, keeping the selenization process the same for all samples.

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References

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