Band alignment engineering at the absorber/buffer heterojunction in kesterite solar cells

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Abstract

Kesterite-based solar cells still suffer from limited efficiency due to various problems related to the absorber and device interfaces. Absorber defects and non-ideal band alignment at the absorber/buffer heterojunction, resulting in a cliff-like conduction band offset (CBO), are the main factors limiting efficiency. Partial and/or complete cation substitution in kesterite represents an emerging strategy to increase efficiency and reduce absorber defects.

This study explores the effect of partial substitution of zinc (Zn) in pure sulfide keserite (Cu2ZnSnS4) by the incorporation of cadmium (Cd) and manganese (Mn). Thin films of Cu_2ZnSnS_4 (CZTS), $Cu_2Zn_{1-x}Cd_xSnS_4$ (CCZTS) and $Cu_2Zn_{1-x}Mn_xSnS_4$(CMZTS) were obtained by chemical solution process. The influence of Cd and Mn incorporation on the morphology, structure, optical and electronic properties of the films was investigated by comparing the pure CZTS with CCZTS and CMZTS. Thin films of CZTS, CCZTS and CMZTS were characterized using scanning electron microscopy (SEM), X-ray diffraction (XRD), UV/Visible spectroscopy, and X-ray photoelectron spectroscopy (XPS). The results indicate an improvement of morphology as well as an adjustment of the band gap and the valence band position with partial substitution of Zn by Cd and Mn.

Moreover, the band alignment at the absorber/buffer heterojunction was investigated using partial Zn substitution. CZTS, CCZTS and CMZTS were used as absorbers and CdS as buffer in a heterojunction prototype. The band alignments at the hetero interface absorber/buffer were evaluated by XPS and UV/Visible measurements [1]. The results show a cliff-like CBO for CZTS/CdS heterojunction, a spike-like CBO for CCZTS/CdS and a near flat-band CBO for CMZTS/CdS heterojunction.

This work shows that Mn offers a non-toxic and reliable Zn substitution strategy to address the heterointerface issue in the pure sulfide kestersite solar cells.

[1] C. Tamin et al., Estimation of band alignment at CdS/Cu_2ZnSnS_4 hetero-interface by direct XPS measurements, Surf Interface Anal. (2020) sia.6881. https://doi.org/10.1002/sia.6881.

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