Optimizing the band offsets of transparent conducting $Zn_{1-x}Sn_xO_{1+\delta}$ alloy to wide-gap $Cu(In,Ga)Se_2$ via oxygen stoichiometry control

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Abstract:

Zinc-Tin-Oxide (ZnSnO, ZTO) has recently drawn much interest as one of the most promising alternative Cd-free buffer material for current state-of-the-art thin film $Cu(In,Ga)Se_2$ (CIGSe) solar cells, due to its non-toxicity and earth-abundance. Meanwhile, the multi-phases of Tin-based oxides, namely Tin dioxide (SnO_2) and Tin monoxide (SnO), as well as the intermediate phases Sn_2O_3 and Sn_3O_4 between them [1], can significantly affect the properties of the resulting ZTO alloy, and hence the band offsets to CIGSe. As such, controlling the oxygen stoichiometry in ZTO alloy is of crucial importance to achieve a favorable bandgap and band offsets to CIGSe. While a moderate spike conduction band (CB) offset of buffer/CIGSe has been reported to effectively mitigate interfacial recombination and thus enhance the open circuit voltage (V_{OC}) in CIGSe solar cells [2], our previous work found that the bandgap of $Zn_{1-x}Sn_xO$ alloy varies from 3.85 eV down to 3.15 eV by adjusting the Sn content x and achieved a CB offset of ~0.2 eV to CIGSe with bandgap of ~1.4 eV at near-mid alloy compositions, as shown in Fig. 1. In this work, we experimentally investigate the effects of oxygen stoichiometry in ZTO alloys on their band offset to a thermal co-evaporated CIGSe. In particular, amorphous $Zn_{1-x}Sn_xO_{1+\delta}$ thin films with $0.2<x<0.6$ are grown by RF reactive co-sputtering at room temperature using 3 targets, namely ceramic ZnO and SnO_2 targets and a metallic Sn target, with the modulating oxygen partial pressure (O_{pp}) in the reactive gas. We first explore the desirable O_{pp} range for the synthesis of stoichiometric SnO and SnO_2, and then select a few O_{pp} values in between for different ZTO compositions within $0.2<x<0.6$. We further carry out post-growth annealing at low temperatures of <300^{o}C to optimize the electrical properties of the ZTO films. We found that $Zn_{1-x}Sn_xO_{1+\delta}$ films sputtered with O_{pp} between SnO and SnO_2 are all amorphous, consistent with the high crystallization temperature of >500^{o}C for Sn_2O_3/Sn_3O_4 and Zn_2SnO_4, all films exhibit an n-type conductivity and visible transparency of >85% with a wide transmission window of >2500 nm after annealing at 300^{o}C. The bandgap and the valence band position are obtained by spectroscopic ellipsometry and ultraviolet spectroscopy, respectively. We anticipate that an optimized $Zn_{1-x}Sn_xO_{1+\delta}$ buffer layer sputter grown on a wide-gap CIGSe with a type I band offset can diminish the undesirable interfacial defects and thus recombination rate in CIGSe solar cell, which will be explored in future work.

Keywords—Cu(In,Ga)Se₂; Zinc-Tin-oxide; band offset

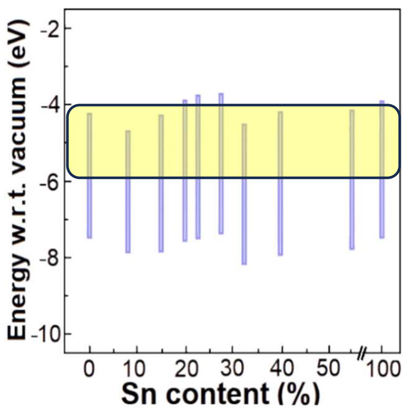

Fig.1 Band offset of $Zn_{1-x}Sn_xO$/CIGSe.

Reference:

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