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Investigation of Ti-based barrier layers for application in monolithic Silicon-Chalcogenide tandem solar cells

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Abstract: Chalcogenides, such as Cu$_2$ZnSnS$_4$ (CZTS), made of environmentally friendly and earth abundant elements are promising materials to be used as the high-bandgap material for silicon-based tandem solar cells. Although there have been large efforts in developing an efficient top cell chalcogenide material, present understanding on the monolithic integration with a silicon cell is very limited. Therefore, an in-depth study to provide insight into the possible interactions of the two materials and the requirements for any intermediate layer between the two cells is essential.

In this work, we have done a systematic study on the possible effects of CZTS growth on the silicon bottom cell. We investigated the performance of different ultrathin (< 25 nm) Ti-based layers, namely TiN, TiN-Al-TiN, and TiO$_2$, as promising barrier materials to protect the silicon cell during the sulfurization process. In this respect, we examined in detail the indiffusion of impurities into Si during the sulfurization of CZTS, in the presence and absence of the barrier layers. Samples without any barrier layer suffered from delamination after the annealing dissimilar to the protected ones. TOF-SIMS measurements revealed that the TiN layer could effectively block in-diffusion of impurities into the silicon substrate. Minority carrier lifetime measurement was used as a figure of merit to determine the effect of trace impurities on the photovoltaic properties of the bottom cell. Even though a slight decrease in lifetime was observed after the CZTS synthesis on Si, an ultimate lifetime of ~1.6 ms was measured indicating promising implied $V_{oc}$ of 707 mV for the bottom cell. This shows that fabrication of a CZTS cell on a silicon cell does not necessarily compromise the performance of the silicon cell. Finally, the actual effect of these layers on the performance of a single-junction silicon solar cell is tested, and the optical and electrical losses due to the presence of the barrier layers as well as to the CZTS processing are discussed.

Keywords: Tandem; Multi-Junction; CZTS; Barrier Layer; Silicon, Chalcogenides