Performance evaluation of WS2 as buffer and Sb2S3 as HTL in CZTS solar cell by numerical simulation

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Abstract

This study reports on performance enhancement in a solar cell introducing Sb2S3 as hole transport layer (HTL)along WS2 as buffer layer. We have investigated photovoltaic (PV) characteristics by utilizing SCAPS-1D. A comparative observation on PV performances of conventional CZTS/CdS with proposed CZTS/WS2 and Ni/Sb2S3/CZTS/WS2 /FTO/Al solar cells is presented. It is revealed that "spike like" band structure at CZTS/WS2 interface having smaller conduction band offset makes it potential alternative to commonly used CdS buffer. This study also evaluates that Sb2S3 as an HTL proposed at back of CZTS enhances performances by reducing carrier recombination at back interface with appropriate band alignment. The impacts of thickness, carrier concentration of different layers, and bulk defect density in CZTS as well as defects at interfaces on performances are analyzed. The influences of temperature, work function as well as cell resistances are also explored. Optimum absorber thickness of 1.0 μm along doping of 10 17 cm-3 is selected. A maximum efficiency of 30.63% is achieved for the optimized CZTS cell. Therefore, these results suggest that Sb2S3 as HTLand WS2 as buffer layer can be employed effectively to develop highly efficient and low-cost CZTS solar cells.

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