Abstract

Quaternary chalcogenide semiconductors may be sustainable and environment-friendly alternative absorber materials to accelerate thin film photovoltaic technology. This work primarily focuses on sol-gel derived spin coating technique for synthesizing Cu_2ZnSnS_4 (CZTS) thin films. A suitable combination of precursors and their chemistry is investigated and the process is optimized for forming the stable sol. CZTS thin films are prepared using optimized sol solution and spin coating. The spin-coated films are thermally treated at different temperature with and without sulfur environment to achieve the phase purity and stoichiometry of CZTS thin films. The fabricated CZTS absorber films are investigated in terms of their structural optical and electrical characteristics for possible improvement in their photovoltaic response. ^{119}Sn Mossbauer measurements are carried out to confirm the site disorder and valence state of tin present in the prepared CZTS films. Mössbauer measurements confirm the IV+ state, however, Sn site disorder is observed for low temperature annealed CZTS, which reduced drastically for high temperature annealed CZTS material. Sn site disorder is correlated with CZTS electronic properties to identify the probable defect states. CZTS solar cell device structure (AZO/i-ZnO/n-CdS/CZTS/Mo/SLG) is fabricated and the synthesis of constituent material layers for the solar cell structure is also discussed in terms of their growth and material properties. Capacitance-voltage and impedance characteristics are investigated for these fabricated solar cells and a resistor-capacitor equivalent circuit is used to analyze the observed photovoltaic response.

Further, one-dimensional simulation is carried out to quantify the impact of various material properties such as carrier concentration, defect density, layer thickness and the quality of heterointerfaces for single junction simulation of CZTS/Se heterostructure solar cell. Further, a dual junction tandem cell structure is proposed and investigated for possible improvements in kesterite based solar devices to realize the high efficiencies. The work also explores new/alternative absorber materials such as CZGS/Se compound semiconductors computationally. The detailed structural, optical and electronic properties are calculated using density functional theory in both kesterite and stannite crystallographic phases. The electronic band gap values are 2.1 eV and 1.77 eV for kesterite phase CZGS and CZGSe. The low and high band gap CZGSe and CZGS compound semiconductors may be very useful materials for designing a single junction and tandem junction solar cells.

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