Abstract

The solar cell has emerged as a newer and a relatively sustainable energy source, that is eco-friendly and cost-effective if the production is on a larger scale. In the current scenario, the economic and high-power conversion efficiency photovoltaic devices without degradation of materials are designed for the generation of electricity. The silicon-based solar cells dominated the market for many years. For the manufacturing and production of silicon-based solar cells, sophisticated fabrication techniques are required that make the solar panel costly. Due to intensification in manufacturing capabilities, thin film solar cells are gaining significance. Thin film technology is one of the most cost-effective and efficient technologies for the manufacturing of solar cells, and it is an excellent subject of intense research in the photovoltaic industry. Thin film technology is economical than other technologies because devices have relatively less material and are based on various types of light absorbing semiconductor materials. Among these materials, kesterite solar cells utilizing $CZTS, CZTSe$ and their alloys $CZTSSe$ are emerging as the most auspicious replacement for the chalcopyrite absorbers. The outstanding electrical and optical features having direct optical band gap ranges among $1.4eV$ to $1.5eV$ and large absorption coefficient $\alpha > 10^4 cm^{-1}$ of CZTS have made it very interesting in the thin film community. According to the Shockley-Queisser limit, the optimum conversion efficiency of around 28 % is theoretically possible from a $CZTS$ based solar cell by tuning the band gap, but still, it is not experimentally possible to achieve 28% conversion efficiency from a solar cell due to lack of understanding of device characteristics. For a better understanding of device characteristics, numerical modeling can play a significant role by modeling different device structures that can save time and cost of the research community. In this work, numerical modeling was carried out for estimating and analyzing the effect of physical parameters such as thickness and doping concentration of absorber, buffer and window layers, temperature effect and effect of illumination power of the sun on device performance. Device modeling had performed on the dedicated simulation software "Solar Cell Capacitance Simulator" ($SCAPS-1D$). To achieve this task first, a simple $p-n-n^+$ structure for $Mo/CZTS/CdS/ZnO/FTO$ had been analyzed with molybdenum as back contact and FTO as a front contact. Through analysis, it had been found that solar cell performance was affected by variation in absorber thickness, doping concentration, and metal work function. After visualization of a basic device structure in $SCAPS-1D$, $CZTS$ based

experimental solar cell had been modeled. Experimentally designed $CZTS$ solar cell results were first simulated in $SCAPS-1D$ environment. The $SCAPS-1D$ simulated results were then compared with experimental results. After optimization of cell parameters, the conversion efficiency of an optimized device was increased and from modeling, it had been found that device performance was improved by improving minority carrier lifetime and integration of back surface field at the back contact. Based on the results presented, it was found that recombination in a solar cell can greatly affect the performance of a solar cell. Therefore, a new structure (Back contact$/CFTS/ZnS/Zn(O,S)/FTO$) was modeled and analyzed in which interface recombination is reduced by optimizing the band gap of $Zn(O,S)$ layer. Based on different device structure modeling, it was found that solar cell with structure $CFTS/ZnS/Zn(O,S)/FTO$ can exhibit an efficiency of 26.11% with optimized physical parameters like absorber thickness layer of $4\mu m$ and acceptor concentration density of $2\times10^{18}\ cm^{-3}$. The proposed results will give a valuable guideline for the feasible fabrication and designing of high-power conversion efficiency solar cells.