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Simulation of the role of defects on the photovoltaic performance of kesterite solar cells

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ABSTRACT

Owing to the reduced toxicity and greater abundance of their constituent elements, Kesterite-based solar cells are attracting considerable attention in recent years. The one-dimensional solar cell capacitance simulator SCAPS-1D has been used for the simulation of single junction solar cells using $Cu_2ZnSnSe_4$ as the absorber layer material. Research has been done on the photovoltaic performance in relation to charge variations and defect density. It has been determined that in order to achieve increased solar efficiency, the light absorbing layer defects must be decreased to a likely lesser concentration. It has also been discovered that the charge of the defects plays a major influence in determining how well the solar cells work.

Keywords: CZTSe, Kesterite Solar Cells, Defects, Simulation, SCAPS-1D.

1. INTRODUCTION

The use of kesterite minerals as light-absorber components in thin-film solar cells has shown great promise. Their attributes, including their high absorption coefficient, earth abundance, cost-effectiveness, non-toxicity, and optimal direct bandgap, have made them a viable alternative to other modern thin-film materials like CdTe and CIGS.. Furthermore, kesterite material satisfies the requirements for solar cells with high efficiency [1]. The Shockley–Queisser limit [2] suggests that its broad bandgap in the range of 1.0 to 1.5 eV (by modifying ratio of S/Se) provides a theoretical maximum efficiency between 20% to 30%. It is also possible to get a larger bandgap of ≈1.7 eV for tandem top cell configuration through element substitution [3].

Keterites are complex quaternary systems that naturally feature low formation energy compensated defect clusters and a variety of point defects [4, 5]. Certain defects are harmful deep-level defects which can function as recombination sites in the bandgap, trapping the photogenerated charge carriers and decreasing the lifetime of the minority charge carrier. Optically bandgap shrinkage and local composition inhomogeneity might result from atom exchange with the environment caused by a high population of

deleterious defect clusters [5, 6]. Thus, controlling absorber layer defects is essential to producing high-efficiency kesterite based solar cells.

In order to comprehend the impact of the charge and density of defects in the light-absorbing CZTSe layer on the performance of solar cells, as well as to determine the ideal defect concentration for achieving the best photovoltaic performance in CZTSe solar cells, we have simulated CZTSe based solar cells with the help of SCAPS-1D simulation software. The necessary required parameters for the various materials used in the simulation approach in the current work have been gathered from the literature and cited appropriately.

2. Material Properties and Simulation Approach

CZTSe serves as the p-type absorber layer in the device structure under consideration, CdS as the n-type buffer layer with wide band gap, ZnO serves as a window and passivation layer, and ZnO doped with Al (Al:ZnO) serves as a transparent conducting oxide (TCO) layer. The device structure is depicted in Fig 1. Table 1 provides an overview of the material properties and is used for simulating the photovoltaic response for the suggested device form [7–11].

Setting the appropriate boundary conditions at the interfaces as well as at the contacts, coupled Poisson and continuity equations for both holes and electrons are numerically elucidated [12–15] in order to model the suggested device designs using the SCAPS-1D [19].

With CZTSe serving as the material for light absorbing layer, this structure—Al:ZnO/ZnO/CdS/Absorber layer/Back contact—is taken into account while simulating single junction solar cells. In addition to supplying the electrical contact at front, Al:ZnO is transparent to the solar radiation incident on the device. P-type CZTSe absorber layer forms a p-n junction heterostructure with window ZnO layer and as buffer n-type CdS layer . Defects are induced in the absorber layer with a single energy distribution at 0.6 eV above E_v. To determine the mid-gap defect, the defect energy level is taken into account. For the back contact, flat band consideration has been taken with speed of surface recombination to be ~ 1 x 10^5 cm s^{-1} and 1 x 10^7 cm s^{-1} for electrons and holes, respectively. Every simulation was run with AM1.5 G 1SUN illumination.

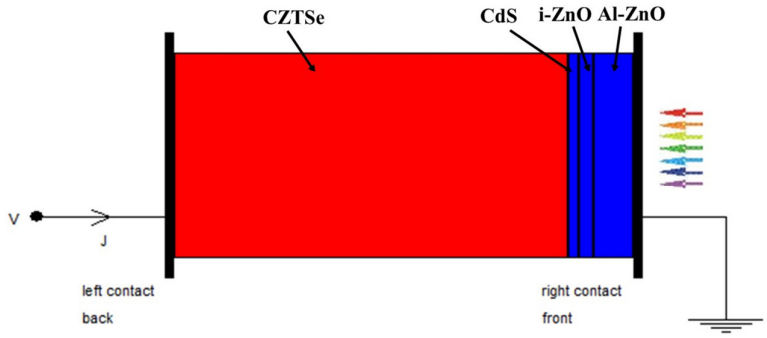

Figure 1: Structure of ***"Al-ZnO/i-ZnO/CdS/CZTSe/Back contact"*** solar cell, studied for simulation of the device performance

Table 1: Materials related parameters used in the present work for the simulation of solar cell structures

	CZTSe	CdS	i-ZnO	Al-ZnO
Thickness (µm)	2	0.05	0.080	0.2
Electron Affinity (eV)	4.46	4.5	4.6	4.6
Bandgap (eV)	1	2.42	3.37	3.37
Dielectric Permittivity	9.1	9	9	9
CB Effective DOS (cm^{-3})	2.2×10^{18}	1.8×10^{19}	2.2×10^{18}	2.2×10^{18}
VB Effective DOS (cm^{-3})	1.8×10^{19}	2.4×10^{18}	1.8×10^{19}	1.8×10^{19}
Hole Thermal Velocity (m/s)	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}
Electron Thermal Velocity (m/s)	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}
Hole Mobility (cm^2/Vs)	40	50	25	25
Electron Mobility (cm^2/Vs)	145	160	150	150
Shallow Uniform Acceptor Density NA (cm^{-3})	5×10^{16}	0	0	0
Shallow Uniform Donor Density ND (cm^{-3})	0	1×10^{17}	1×10^{17}	1×10^{20}

3. Results and Discussion

It was observed that the light absorbing CZTSe layer, which is composed of donor and acceptor vacancies, interstitials, and antisites, is susceptible to defects due to the effect of defect charge and concentration [16]. Without the addition of an external dopant element, the CZTSe is naturally p-type semiconductor because to its low formation energy acceptor defects. Different kinds of charged defects can be introduced via SCAPS [17–19]. The present study examines charged defects with a distinctive energy level of 0.6 eV, which is situated exactly above the valance band. The minority charge carriers' lifetime in the absorber layer is determined by the concentration of bulk defects [20]. Table 2 provides a summary of the changes in short circuit current density, open circuit voltage, photovoltaic efficiency, and fill factor versus various defect concentrations in the light absorbing layer. It is noted that open circuit voltage, short circuit current density, efficiency, and fill factor do not significantly alter with decreasing absorber layer defect concentrations. This might be because the defect photogenerated charge carriers are less scattered due

to a lower defect concentration, which has no impact on the device's functionality. However, a sharp decline in efficiency is shown for the CZTSe absorber layer, nearly to zero for the defects of donor type, when the defects concentration is increased to a specific higher concentration of 10^{17} cm^{-3}. Table 2 makes this decline in fill factor, open circuit voltage, solar efficiency, and short circuit current density very evident. Furthermore, it can be inferred that the introduction of donor type defects in the kesterite absorber layer results in the highest reduction in efficiency, also at high defect concentrations near 10^{17} cm^{-3}. In order to achieve higher solar efficiency, defects in the light absorbing layer must be diminished to the lowest feasible values, and their charge type must also be managed [21].

Table 2: Performance parameters for the solar cell device at various concentrations of defect as calculated by SCAPS

	Concentration of Defects	**J_{sc}**	**V_{oc}**	**FF**	**η**
Without Defects		26.08	0.52	80.06	11.03
Neutral Defects	**10^{14}**	26.06	0.52	80.03	11.01
	10^{15}	25.89	0.52	79.44	10.83
	10^{16}	24.41	0.51	77.28	9.68
	10^{17}	17.62	0.45	67.29	5.42
	10^{18}	9.84	0.32	56.59	1.81
	10^{19}	5.81	0.18	48.59	0.51
	10^{20}	3.47	0.07	37.08	0.1
Single Donor Defects	**10^{14}**	26.06	0.52	80.02	11.01
	10^{15}	25.90	0.52	79.4	10.82
	10^{16}	24.58	0.50	76.15	9.48
	10^{17}	5.82	0.03	26.34	0.06
Single Acceptor Defects	**10^{14}**	26.06	0.52	80.03	11.01
	10^{15}	25.89	0.52	79.44	10.83
	10^{16}	24.41	0.51	77.3	9.69
	10^{17}	17.60	0.54	67.95	5.49
	10^{18}	9.73	0.35	58.51	2.01
	10^{19}	5.520	0.24	51.28	0.7

4. Summary and Future Prospective

With the PV market continuing to grow, kesterites CZTSSe solar cells, which are mostly composed of green materials and have low manufacturing costs, are becoming more and more attractive for large-scale deployment. The simulation software SCAPS-1D has been used to study solar cells based on kesterite (CZTSe). By lowering the defects concentration and managing their type of charge, the suggested cell structure shows promise for improving the solar cell efficiency with absorber layers based on kesterite materials. The current study demonstrated that single junction CZTSe solar cell architectures have an optimal efficiency of roughly 11%. The current study has demonstrated that a reasonable level of concentration of defects in the absorber layer is necessary to obtain greater efficiency in s solar cell with ingle junction architectures. In conclusion, it is necessary to reduce flaws and defect clusters since they are particularly undesirable in kesterite materials. The best bandgap grading profile with intentional control and excellent reproducibility can be investigated further as a means of improving the photovoltaic efficiency of kesterite materials based solar cells.

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