

Research Article

Non-Toxic Buffer Layers in Flexible Cu(In,Ga)Se₂ Photovoltaic Cell Applications with Optimized Absorber Thickness

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Absorber layer thickness gradient in Cu(In_{1-x}Ga_x)Se₂ (CIGS) based solar cells and several substitutes for typical cadmium sulfide (CdS) buffer layers, such as ZnS, ZnO, ZnS(O,OH), Zn_{1-x}Sn_xO_y (ZTO), ZnSe, and In₂S₃, have been analyzed by a device emulation program and tool (ADEPT 2.1) to determine optimum efficiency. As a reference type, the CIGS cell with CdS buffer provides a theoretical efficiency of 23.23% when the optimum absorber layer thickness was determined as 1.6 μm. It is also observed that this highly efficient CIGS cell would have an absorber layer thickness between 1 μm and 2 μm whereas the optimum buffer layer thickness would be within the range of 0.04–0.06 μm. Among all the cells with various buffer layers, the best energy conversion efficiency of 24.62% has been achieved for the ZnO buffer layer based cell. The simulation results with ZnS and ZnO based buffer layer materials instead of using CdS indicate that the cell performance would be better than that of the CdS buffer layer based cell. Although the cells with ZnS(O,OH), ZTO, ZnSe, and In₂S₃ buffer layers provide slightly lower efficiencies than that of the CdS buffer based cell, the use of these materials would not be deleterious for the environment because of their non-carcinogenic and non-toxic nature.

1. Introduction

Solar cells based on thin-film CuInSe₂ (CIS) and Cu(In_{1-x}Ga_x)Se₂ (CIGS) absorbers have major contributions in photovoltaic technology due to their lower cost, flexible modules, and high energy conversion efficiency of more than 21% [1–4]. The absorber works as a p-type doped area into a CIS and CIGS model with a typical thickness of 1–2 μm [5]. For the CIS absorber layer, the band gap is about 1 eV (0.98–1.04 eV) [6]. By introducing the gallium content, [Ga]/([Ga + In]), into the CIS absorber, the band gap of CIGS can be varied from 1.04 to 1.7 eV [4] although the optimal band gap of CIGS ranges from 1.16 eV to 1.38 eV due to the Ga grading in the CIS absorber [7–10]. To show the effects of absorber band gap on the properties of the CIGS solar cell, in this study, the CIGS band gap is optimized as 1.25 eV for [Ga]/([Ga + In]) = 0.45 [11]. While growing CdS buffer on the CIGS absorber, the critical thickness of the CdS buffer layer was found to be around 50 nm.

Besides this, the chemical bath-deposited (CBD) ZnS buffer layer having a wider band gap ($E_g = 3.68$ eV) has shown the second highest efficiency in the thin-film technology for the replacement of CdS [12]. Atomic layer-deposited (ALD) Zn_{1-x}Sn_xO_y (ZTO) has also been used for the replacement of CdS, and the best cell efficiency of the CIGS solar cell with a ZTO buffer layer has been recorded as 18.2% [11]. The wider band gap of ZTO is used as it permits transmitting the photons having lower wavelength into the absorber. Hence, the current generation is also increased owing to using ZTO as a buffer. Zinc oxide, ZnO, is also used as an alternative to the CdS buffer layer as it has a band gap of 3.30 eV, which is 0.88 eV wider than that of CdS ($E_g = 2.42$ eV). But with the ZnO buffer layer, the cell does not show the light-soaking effect [13]. During the heteroepitaxial growth of the buffer layer using the atomic layer deposition (ALD) technique, the existence of the effect is realized. This effect is primarily associated with the surface properties of the CIGS absorber. To subside the light-soaking effect, the CIGS

TABLE 1: Material parameters for CIGS solar cell simulation.

Parameters	ZnO:Al	i-ZnO	CdS	CIGS
Thickness, τ (μm)	0.2	0.02	0.05	1
Dielectric constant, E_{ps}	7.8	7.8	12	13.6
Refractive index, N_{dx}	2	2	3.15	3.67
Band gap, E_{g} (eV)	3.30	3.30	2.42	1.25
Electron affinity, χ_{e} (eV)	4.6	4.6	3.74	4.19
Donor concentration, N_{d} (cm^{-3})	5×10^{16}	1×10^{17}	3×10^{16}	0
Acceptor concentration, N_{a} (cm^{-3})	0	0	0	2×10^{16}
Electron mobility, μ_{n} ($\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$)	100	100	120	110
Hole mobility, μ_{p} ($\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$)	25	25	40	35
Conduction band effective density of states, N_{c} (cm^{-3})	2.2×10^{18}	2.2×10^{18}	2.2×10^{18}	2.2×10^{18}
Valence band effective density of states, N_{v} (cm^{-3})	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}

TABLE 2: Base parameters of the substitute buffer layers.

Parameters	ZnO	ZnS	ZnS(O,OH)	$\text{Zn}_{1-x}\text{Sn}_x\text{O}_y$	ZnSe	In_2S_3
τ (μm)	0.03	0.04	0.05	0.05	0.04	0.05
E_{g} (eV)	3.30	3.68	3.80	3.74	2.71	2.90
χ_{e} (eV)	4.60	4.13	4.24	4.06	4.09	3.85
N_{d} (cm^{-3})	1×10^{17}	5×10^{16}	1×10^{17}	1×10^{17}	2×10^{17}	1×10^{17}
μ_{n} ($\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$)	100	250	200	160	60	400
μ_{p} ($\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$)	30	70	60	40	20	120

surface is doped or etched with Zn, and hence, the solar cell with the ALD technique yielded an efficiency of 13.9% [14]. Besides the CdS, ZnS, and ZnO based buffer layers, we also investigate the properties of ZnSe, In_2S_3 , and ZnS(O,OH) buffer layers and their effects on the CIGS solar cell performance.

2. Experimental

ADEPT 2.1 (a device emulation program and tool: version 2.1) is a one-dimensional online simulator to analyze the electrical and optical characteristics of silicon based solar cells, CIGS and CdTe based thin films, GaAs solar cells, and so on [15]. In this paper, ADEPT 2.1 was used to simulate and investigate CIGS solar cell properties with different buffer layers. Current-voltage characteristics in light and dark conditions can be achieved from the simulation carried out by ADEPT 2.1 simulation. For all the solar cell structures, quantum efficiency, J - V characteristics, electric field, current generation, saturation current, energy band gap profile, and so on are measured as a function of light bias, voltage, or temperature. Moreover, from the ADEPT 2.1 simulation, recombination profiles, carrier concentration, electric field distributions, and carrier current densities can be obtained as a function of thickness. However, the properties of the conventional CdS and its alternative materials such as ZnO, ZnS, ZnS(O,OH), ZTO, ZnSe, and In_2S_3 and their effects on the performance of the n-ZnO/i-ZnO/buffer/CIGS solar cell are emphasized in this study. The

analytical aspects are observed due to the changes in efficiency (η), open-circuit voltage (V_{oc}), short-circuit current (J_{sc}), and fill factor (FF). The effects of CdS buffer layer thickness, the various buffer layer material parameters, and the CIGS absorber thickness are also taken into account during the simulation. The base parameters for the CIGS cell structure with CdS buffer used for the simulation are shown in Table 1 [1, 3, 4, 11, 16, 17]. The most important parameters of different buffer layer materials needed for the simulations are depicted in Table 2 [4, 17–31].

3. Results and Discussions

3.1. Effects of Absorber Thickness on CIGS Cell Performance. To make the simulation reasonable, the conventional CIGS thin-film structure has been ascertained in terms of $\text{Cu}(\text{In,Ga})\text{Se}_2$ absorber. Firstly, to determine the optimum thickness of the CIGS cell structure with the most commonly used CdS buffer, the thickness of the CIGS absorber (τ_{absorber}) was varied. In Figure 1(a), it is shown that the open-circuit voltage (V_{oc}) is increasing with varying τ_{absorber} . Figure 1(b) shows that the short-circuit current density (J_{sc}) of the solar cell is also increasing with the increase of τ_{absorber} . Because of being in the p-type area in the cell, V_{oc} and J_{sc} are increased with enhancement of the CIGS absorber layer thickness, τ_{absorber} . This phenomenon permits the photons with longer wavelengths to be accumulated, which in turn leads to generation of electron-hole pair (EHP). It is also easily realized that if τ_{absorber} is decreased, the value of

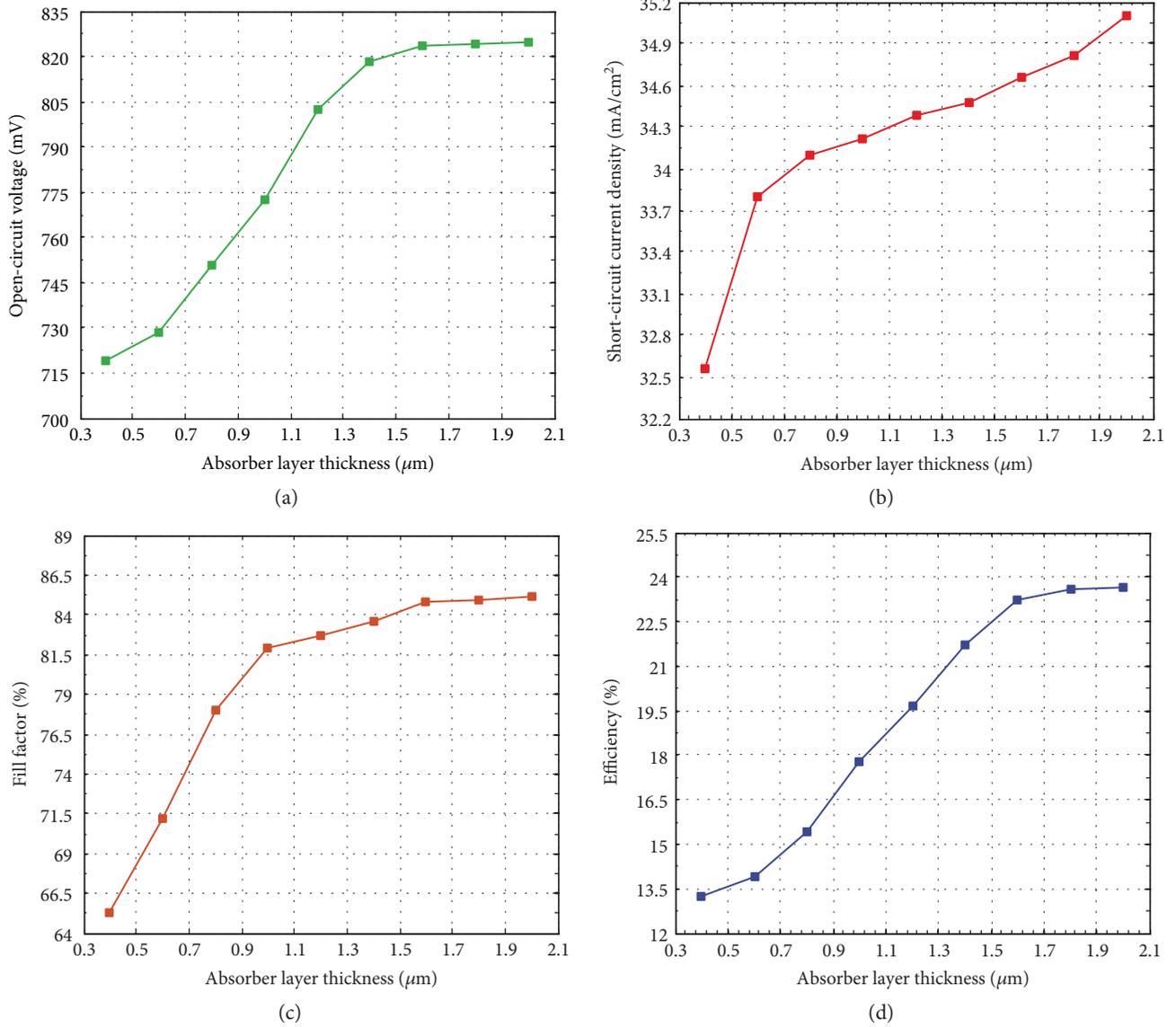


FIGURE 1: Performance variation due to variable thickness of the CIGS absorber layer: (a) open-circuit voltage (V_{oc}); (b) short-circuit current density (J_{sc}); (c) fill factor; (d) efficiency.

both V_{oc} and J_{sc} will be decreased. It is seen from Figure 1(c) that, after $1 \mu\text{m}$, the fill factor (FF) of this simulated CIGS solar cell is almost constant with the τ_{absorber} variation. From Figure 1(d), it is clearly observed that the solar cell efficiency (η) increases with the increase of the CIGS absorber thickness, but over $1.6 \mu\text{m}$, the efficiency variation seems to be very slow. τ_{absorber} would be optimum around $1.6\text{--}2 \mu\text{m}$. The efficiencies were recorded as 17.76% and 23.67% for the thicknesses of $1 \mu\text{m}$ and $2 \mu\text{m}$, respectively. By comparing these results, it is observed that a 5.47% increase in efficiency was found due to the increase of $0.6 \mu\text{m}$ (from $1 \mu\text{m}$) in τ_{absorber} . And an enhancement of $0.4 \mu\text{m}$ from $1.6 \mu\text{m}$ in τ_{absorber} results in only 0.44% increase in efficiency.

The recombination process at the back contact of the cell may cause the enhancement in the values of J_{sc} and V_{oc} . The

back contact will go very close to the depletion area while reducing the absorber layer thickness. Therefore, the back contact captures the electrons for the recombination in an easy way. Hence, a smaller number of electrons contribute to the collection efficiency, and thus, the values of J_{sc} and V_{oc} decrease. Figure 2 shows the J - V characteristic curve with the performance parameters such as V_{oc} , J_{sc} , FF, and efficiency computed after conducting the simulation.

Figure 3 shows the variation in quantum efficiency with respect to photons' wavelengths according to the variation in absorber layer thickness, τ_{absorber} . It is observed that if the thickness of the absorber layer increases, then the quantum efficiency of the solar cell is increased. While increasing the thickness of the absorber layer, a large number of photons are absorbed, including photons

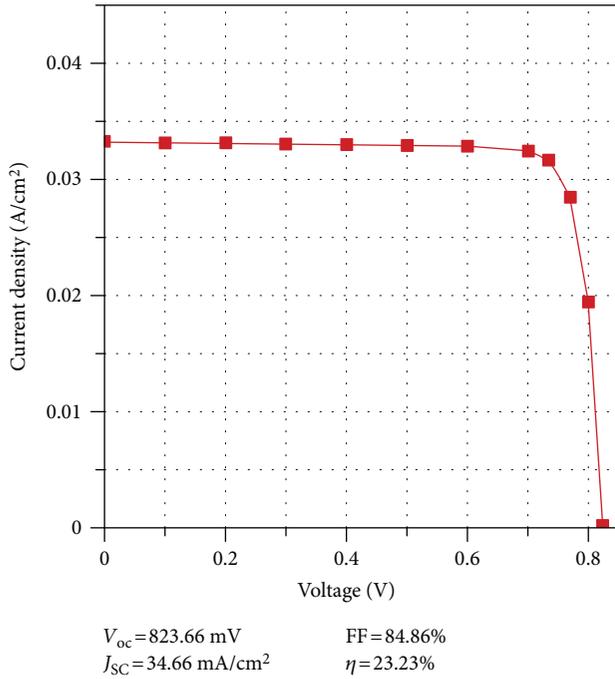


FIGURE 2: J - V characteristic curve with photovoltaic parameters.

having longer wavelengths. The absorbed photons produce a larger number of electron-hole pairs (EHP) in this way. Thus, the increased τ_{absorber} substantiates the increase in external quantum efficiency (EQE).

3.2. Effects of Various Buffer Layers on Cell Efficiency. The six potential buffer layers which have been investigated besides the conventional CdS are ZnS, ZnS(O,OH), ZnSe, ZnO, $\text{Zn}_{1-x}\text{Sn}_x\text{O}_y$, and In_2S_3 . For all cases, the thickness has been varied from $0.01 \mu\text{m}$ to $0.1 \mu\text{m}$. More photons are absorbed by the CdS buffer layer while increasing the thickness of the layer. The optimum thickness of CdS buffer is determined as $0.05 \mu\text{m}$ since J_{sc} decreased dramatically after $0.05 \mu\text{m}$ [32]. However, the ZnS(O,OH) based CIGS solar cell is typically not affected by the thickness of the buffer layer because of the wider band gap of ZnS. It is seen that the efficiencies of the ZnO, ZnSe, and In_2S_3 based solar cells have been decreased when the thicknesses of these layers cross beyond $0.05 \mu\text{m}$. Hence, the optimum thickness of the mentioned buffer layers would be suggested as $0.05 \mu\text{m}$. On the other hand, after the buffer layer thickness of $0.06 \mu\text{m}$, the efficiency of the $\text{Zn}_{1-x}\text{Sn}_x\text{O}_y$ (ZTO) based CIGS cell increases. Figure 4 gives a summary of the simulated J - V characteristic curves with different performance parameters for the CIGS cell based on various buffer layers.

From the simulated results, it is suggested that the ZnO buffer would be a promising alternative to the CdS buffer layer in the CIGS cell as the ZnO and ZnS based cells have reached efficiency levels of 23.67% and 24.62%, respectively. Consequently, ZnO and ZnS are proposed to be very potential materials for conventional CdS replacement because of having wider band gap than that of CdS and higher efficiency than that of the CdS based cell. Although ZTO, ZnS(O,OH), ZnSe, and In_2S_3 based cells provide slightly

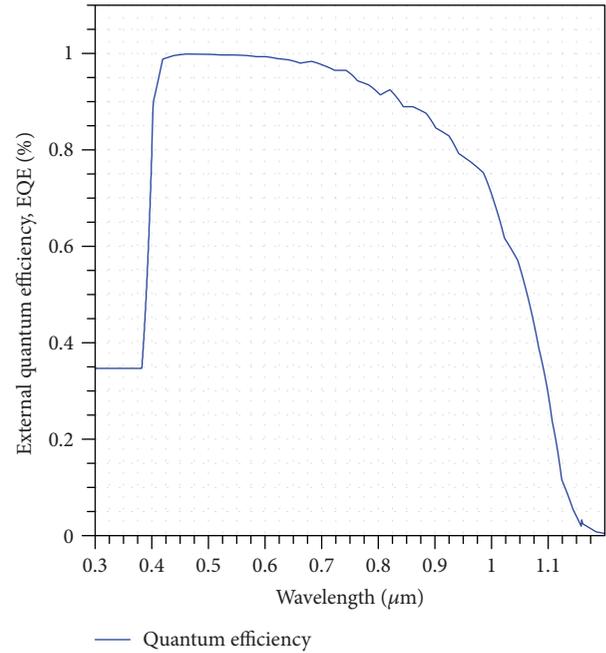


FIGURE 3: Spectral response of CIGS photovoltaic cell.

lower efficiencies than CdS based CIGS solar cells, these materials are nontoxic in nature while the CdS is categorized as carcinogenic and toxic [33]. As a result, these materials can be used as substitute buffer layers for CIGS absorber-based chalcopyrite thin-film photovoltaic devices and will be environmentally friendly enough compared to that of the CdS based cell. The comparisons among different performance parameters of CIGS cells with different substitute buffer layers are shown in Figure 5.

Finally, the comparisons of the improved cell efficiencies for different buffer layers with the relevant experimental results in the literature [1, 11, 12, 17, 34–36] are shown in Table 3.

4. Conclusions

At first, the performance measurements due to the variation in absorber layer thickness in the CIGS solar cell with a CdS buffer layer have been investigated, and thus, the optimum thickness has been figured out from the analysis. Afterwards, various buffer layer materials such as ZnO, ZnS, ZnS(O,OH), ZnSe, ZTO, and In_2S_3 have been used into the CIGS cells. The optimum thicknesses of all the buffer layer materials studied are in the range of 0.04 – $0.06 \mu\text{m}$ whereas the absorber layer thickness was optimized as $1.6 \mu\text{m}$. While comparing the performances of the cells with different buffer layers, it has been observed that the cell with a ZnS buffer layer reveals the highest efficiency of 24.62% among all the cells studied. The second highest efficiency of 23.67% was found from the simulation result of the cell having a ZnO buffer layer. Besides, the comparative analysis of the cells with ZnS(O,OH), ZnSe, ZTO, and In_2S_3 buffer layers also shows a higher efficiency of more than 18%, which asserts the possible replacement of the conventional CdS buffer layer material in CIGS thin-film device structures.

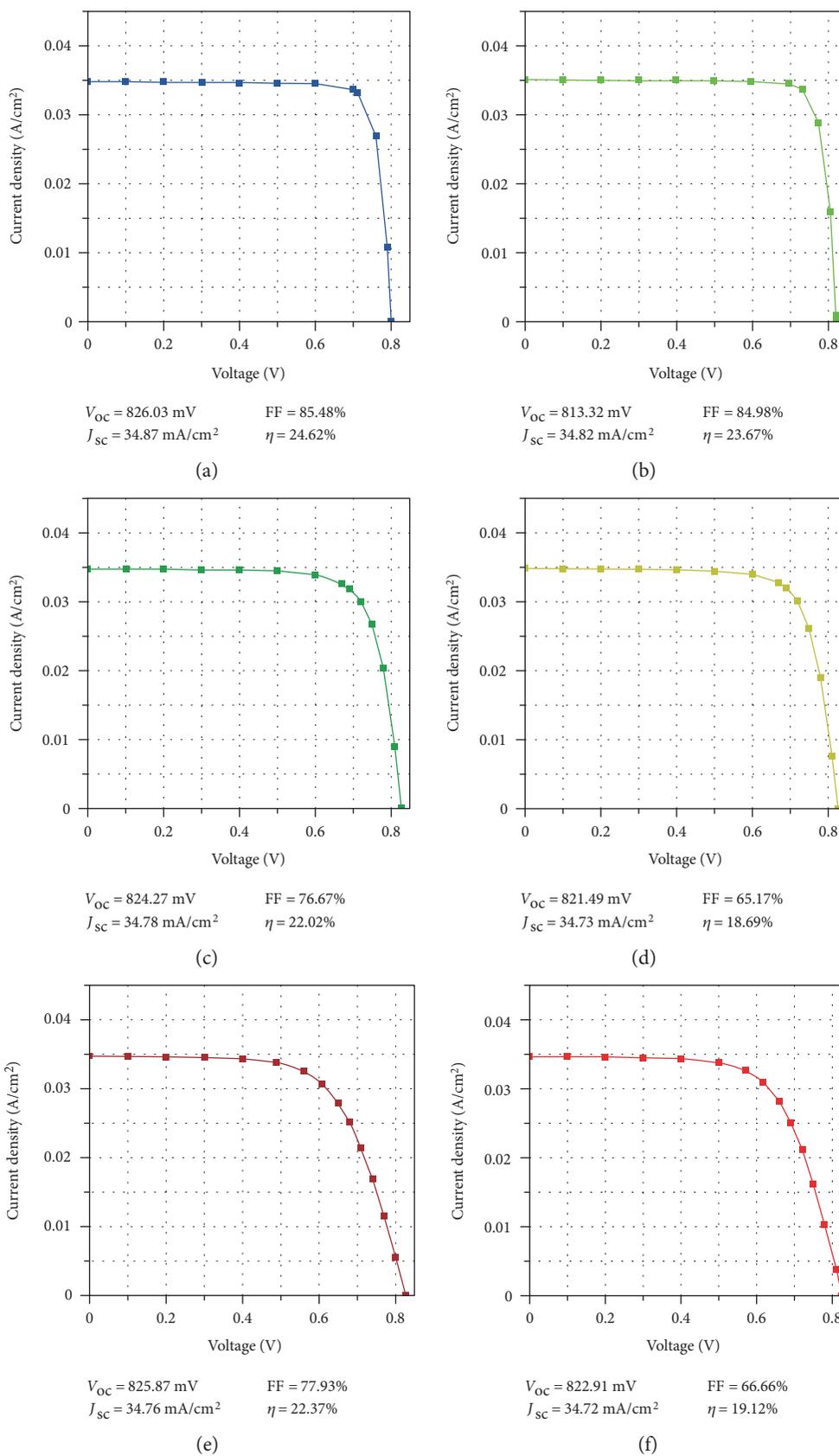


FIGURE 4: *J-V* characteristic curves for CIGS cell with different buffer layers: (a) ZnS; (b) ZnO; (c) ZnS(O,OH); (d) ZnSe; (e) ZTO; (f) In₂S₃.

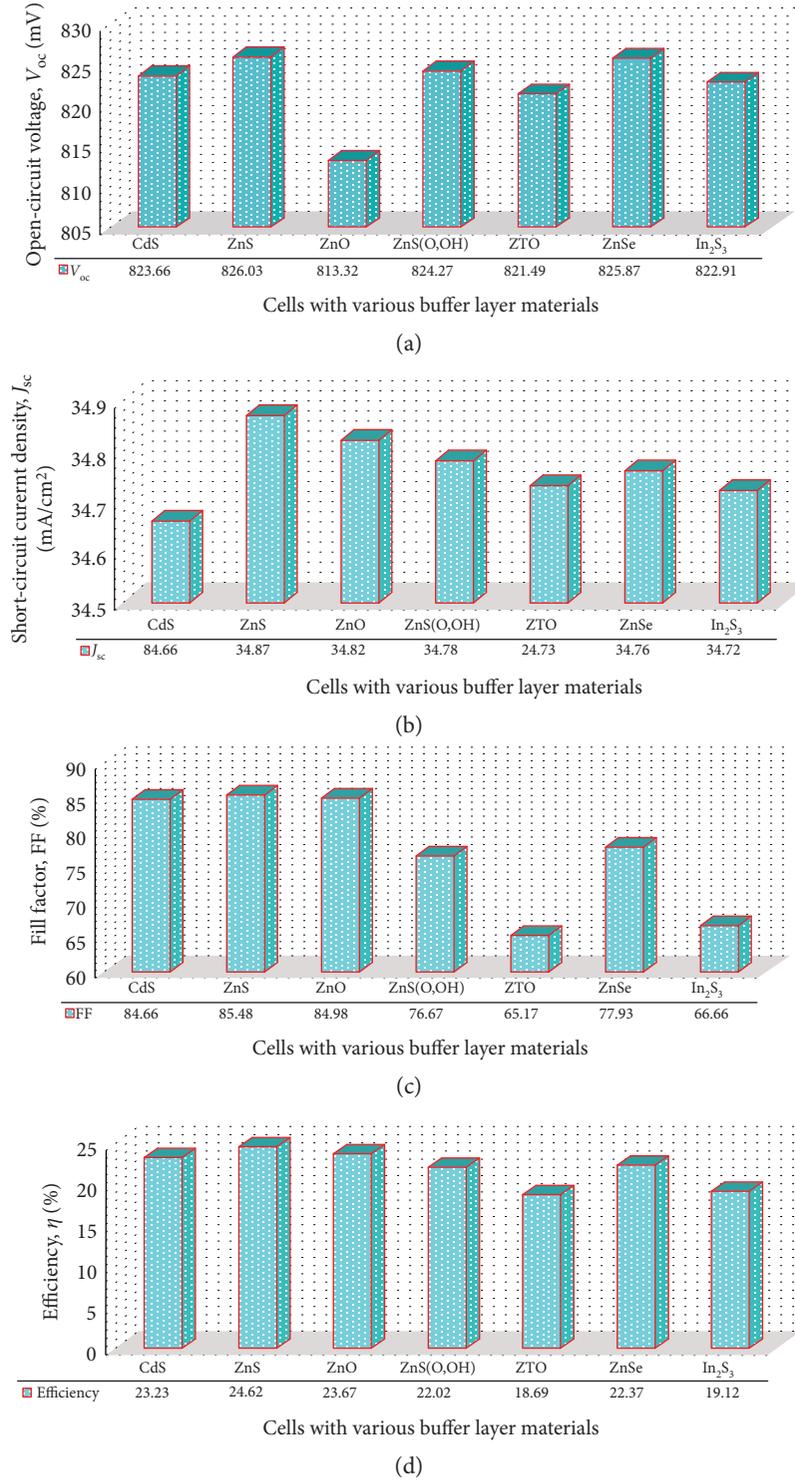


FIGURE 5: Performance comparison among CIGS cells with different buffer layers: (a) open-circuit voltage, V_{oc} ; (b) short-circuit current density, J_{sc} ; (c) fill factor, FF; (d) efficiency, η .

TABLE 3: Comparisons of the improved efficiencies with the relevant experimental results.

Cells	CdS	ZnS	ZnO	ZnS(O,OH)	ZTO	ZnSe	In ₂ S ₃
Proposed cells	23.23	24.62	23.67	22.02	18.69	22.37	19.12
Reference cells	22.60 [1]	18.10 [12]	20.80 [34]	18.40 [35]	18.20 [11]	19.15 [17]	16.40 [36]

Conflicts of Interest

The authors declare that there is no conflict of interest regarding the publication of this paper.

Authors' Contributions

Md. Asaduzzaman conducted the simulation, analyzed the simulation results, and prepared and submitted the manuscript. Md. Billal Hosen and Md. Karamot Ali assisted in conducting the simulation, analyzing the results, and preparing the manuscript. Ali Newaz Bahar supervised the study. All authors finally approved the manuscript for submission.

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