Research Article

Thickness Dependence of Window Layer on CH$_3$NH$_3$PbI$_{3-x}$Cl$_x$ Perovskite Solar Cell

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CH$_3$NH$_3$PbI$_{3-x}$Cl$_x$ has been studied experimentally and has shown promising results for photovoltaic application. To enhance its performance, this study investigated the effect of varying thickness of FTO, TiO$_2$, and CH$_3$NH$_3$PbI$_{3-x}$Cl$_x$ for a perovskite solar cell with the structure glass/FTO/TiO$_2$/CH$_3$NH$_3$PbI$_{3-x}$Cl$_x$/Spiro-OMeTAD/Ag studied using SCAPS-1D simulator software. The output parameters obtained from the literature for the device were 26.11 mA/cm$^2$, 1.25 V, 69.89%, and 22.72% for $J_{sc}$, $V_{oc}$, FF, and $\eta$, respectively. The optimized solar cell had a thickness of 100 nm, 50 nm, and 300 nm for FTO, TiO$_2$, and CH$_3$NH$_3$PbI$_{3-x}$Cl$_x$ layers, respectively, and the device output were 25.79 mA/cm$^2$, 1.45 V, 78.87%, and 29.56% for $J_{sc}$, $V_{oc}$, FF, and $\eta$, respectively, showing a remarkable increase in FF by 8.98% and 6.84% for solar cell efficiency. These results show the potential of fabricating an improved CH$_3$NH$_3$PbI$_{3-x}$Cl$_x$ perovskite solar cell.

1. Introduction

The demand for energy is on an increasing trend. This is characterized by the speedy technological advancement and rapid growth of the economy globally. The world population is also growing rapidly and thus primary sources of energy will be exhausted if an effective alternative source of energy is not sought. The oil reservoirs, coal, as well that of the gas will completely be exploited in the next 35 years, 107 years, and 37 years, respectively [1]. Furthermore, the burning of fossil fuels has significantly contributed to environmental pollution and global warming [2]. Therefore, there is a need to find a clean, renewable, and sustainable alternative source of energy. Solar energy has for a long time been considered among the best alternative source of energy owing to its abundance but harvesting and conversion technology has been the limiting factor. For decades, silicon has remained the dominant material for the production of commercial solar conversion devices. Research seems to suggest that perovskites stand to be good candidates among other materials [3, 4].

Perovskite solar cells (PSCs) have attracted much attention in the field of photovoltaic due to their high light absorption, tunable band-gap energy, high open-circuit voltage, easy synthesis and fabrication, low cost, good thermal stability, and high efficiency [5–8]. In the past 10 years, the efficiency of PSCs has greatly improved from about 2.2% to more than 22% [9]. The understanding of the operational mechanism of the PSCs is necessary for further improvement of its efficiency and thus numerical simulation is a key technique that will enable us to understand the operational mechanisms of PSCs [10]. The simulation will further help prognosticate the maximum value of the solar cell with controlled design. Therefore, the aim of this study was to employ SCAPS-1D software [11] to obtain optimum thicknesses for the window layer and absorber in order to enhance CH$_3$NH$_3$PbI$_{3-x}$Cl$_x$ power conversion efficiency. The interface of layers is known to affect the photovoltaic performance of
the solar cells, but in the present study, its effect was not considered.

1.1. Numerical Model for the Perovskite Solar Cell and Material Parameters. The designing and characterizing of the CH$_3$NH$_3$PbI$_{3-x}$Cl$_x$ PSC model was done using the simulation tool SCAPS-1D version 3.3.07 (“SCAPS3307”) [11]. The SCAPS software has the ability to solve the fundamental semiconductor equations; the Poisson equations, the continuity equations for electrons and holes, and carrier transport [12]. The working point conditions of the SCAPS simulations were temperature 300 K, work point bias voltage 0 V, and frequency of $1.0 \times 10^6$ Hz. The influence of variation of temperature and the surrounding such as moisture of inert gas was not studied. However, as reported by Usha et al. [13], an increase in temperature beyond 300 K would lead to a drastic decrease in the solar cell performance. The simulation was done under AM1.5G 1 sun spec.

The cell structure consists of FTO/TiO$_2$ multilayer films on glass substrate, CH$_3$NH$_3$PbI$_{3-x}$Cl$_x$ absorber layer, a Spiro-OMeTAD hole transport layer, and silver back contact as shown in Figure 1. Fluorine doped tin oxide (FTO) acts as transparent conducting oxide (TCO) as well as the front electrode. Its thickness was varied from 5 nm to 50 nm while maintaining other layer parameters constant. The results obtained are as shown in Figures 4. Figure 4(a) shows open-circuit voltage and short-circuit current density as functions of TiO$_2$ thickness while Figure 4(b) shows the fill factor and solar cell efficiency as functions of TiO$_2$ thickness.

2. Results and Discussion

2.1. Effect of FTO Thickness. A transparent conducting oxide (TCO) plays an important role in a solar cell since it is employed as the front electrode as well as a backside reflector [22]. Therefore, the influence on the variation of FTO thickness on the performance of CH$_3$NH$_3$PbI$_{3-x}$Cl$_x$ PSC was studied. Figures 3 show the analysis of the performance cell, i.e., $V_{oc}$, $J_{sc}$, FF, and PCE of CH$_3$NH$_3$PbI$_{3-x}$Cl$_x$ PSC as functions of FTO thickness varied from 100 nm to 450 nm, while keeping other layer parameters constant.

Figure 3(a) shows that open-circuit voltage does not change with an increase in FTO thickness, whereas short-circuit current density decreases from 26.18% to 26.07% when FTO thickness is increased from 100 nm to 450 nm. The increase in FTO thickness leads to increased optical absorption of incident light in the layer at the front side of the cell which in turn leads to internal scattering, prolonging the path of light [23, 24]. Therefore, the increased absorption leads to a decrease in the amount of photons reaching the absorber layer which reduces the amount of current generated, and consequently the short-circuit current decreases. The constant $V_{oc}$ observed is because the major process in photovoltaic is excitation of charges, which occurs in the absorber layer. The Fermi level splitting within the CH$_3$NH$_3$PbI$_{3-x}$Cl$_x$ absorber layer is within the band edges of FTO, thus $V_{oc}$ of the cell remains constant.

Figure 3(b) shows a negligible improvement of FF from 70.77% to 70.80% as the FTO thickness increase from 100 nm to 450 nm. On the other hand, PCE decreases with an increase in FTO thickness. The decrease in efficiency is associated with a decrease in $J_{sc}$ as explained above. This decrease in $J_{sc}$ can also be explained in terms of charge extraction. The generated charges need to have a longer lifetime to be extracted through the FTO but that is not possible. Consequently, there is an increase in charge recombination occurring at the FTO and at the FTO/TiO2 interface as a result of an increase in diffusion length with an increase in FTO thickness. Therefore, from the above simulation, it is clear that a 100 nm thick FTO will significantly improve the performance of CH$_3$NH$_3$PbI$_{3-x}$Cl$_x$ PSC.

2.2. Effect of TiO$_2$ Thickness. TiO$_2$ plays a key role in the performance of the device in transporting the generated electrons while blocking the holes from reaching the FTO electrode. Its thickness was varied from 5 nm to 50 nm while maintaining other layer parameters constant. The results obtained are as shown in Figures 4. Figure 4(a) shows open-circuit voltage and short-circuit current density as functions of TiO$_2$ thickness while Figure 4(b) shows the fill factor and solar cell efficiency as functions of TiO$_2$ thickness.

It is observed from Figures 4 that there is no significant change in $J_{sc}$, $V_{oc}$, FF, and $\eta$ as TiO$_2$ thickness increases from 5 nm to 50 nm. Although, there were no significant changes observed, a 5-50 nm thick TiO$_2$ gave an average of 26.18 mA/cm$^2$, 1.25 V, 70.77%, and 23.10% for $J_{sc}$, $V_{oc}$, FF, and $\eta$, respectively. The observation implies that the buffer thickness between 5 nm and 50 nm have no much effect on
the device performance. TiO₂ thickness of more than 50 nm may have deteriorating solar cell properties as reported by Odari et al. [20]. Due to fabrication challenges, we chose 50 nm thick TiO₂ as our optimum value which agrees with experimental work [25].

2.3. Effect of CH₃NH₃PbI₃₋ₓClₓ Thickness. The efficiency of the device majorly depends on the absorber thickness, and therefore the cell was simulated to determine the influence of variation in CH₃NH₃PbI₃₋ₓClₓ thickness on open-circuit voltage ($V_{oc}$), short-circuit current density ($J_{sc}$), fill factor (FF), and power conversion efficiency (PCE). CH₃NH₃PbI₃₋ₓClₓ thickness was varied from 100 nm to 1200 nm while keeping other layer parameters constant. The results obtained are as shown in Figures 5. Figure 5(a) shows open-circuit voltage and current density as functions of CH₃NH₃PbI₃₋ₓClₓ thickness, while Figure 5(b) shows the fill factor and efficiency of the solar cell as functions of CH₃NH₃PbI₃₋ₓClₓ thickness.

It is observed from Figure 5(a) that short circuit-current density increases with the increase of CH₃NH₃PbI₃₋ₓClₓ thickness from 100 nm to 300 nm and slightly levels from 300 nm to 1200 nm. The $J_{sc}$ increases rapidly from 24.69% to 26.02% for a thickness from 100 nm to 300 nm. The $J_{sc}$ majorly relies on the production of the charge carriers. The increase of CH₃NH₃PbI₃₋ₓClₓ thickness leads to an increase in the absorbed light and carrier concentration which consequently leads to increment in short-circuit current. The increase in $J_{sc}$ can also be associated with a high absorption coefficient (10¹⁵ cm⁻¹) of the CH₃NH₃PbI₃₋ₓClₓ layer [26]. The flattening of $J_{sc}$ curve after 300 nm implies that at this point all light is absorbed [27]. On the other hand, there is a significant decrease of open-circuit voltage with an increase of CH₃NH₃PbI₃₋ₓClₓ thickness from 100 nm to 1200 nm. The decrease of $V_{oc}$ implies that the absorber thickness increases the recombination current since in thicker absorber devices, carrier charges generated near the centre of CH₃NH₃PbI₃₋ₓClₓ layer recombines when the thickness surpasses the diffusion length. Further, the increase of CH₃NH₃PbI₃₋ₓClₓ thickness leads to the reduction of its effective bandgap which consequently leads to a reduction in $V_{oc}$ [27, 28].

From Figure 5(b), it is observed that the fill factor decreases incessantly from 75.88% to 68.53% as the absorber thickness increases from 100 nm to 300 nm. The $J_{sc}$ curve starts to attenuate around 300 nm, our simulation shows that an absorber thickness from 300 nm to 1200 nm is suitable. Therefore, a 300 nm-thick CH₃NH₃PbI₃₋ₓClₓ, xClₓ layer showed an improved device performance.

The major task of the simulation was to optimize the FTO, TiO₂, and CH₃NH₃PbI₃₋ₓClₓ thicknesses which would give an improved performance of CH₃NH₃PbI₃₋ₓClₓ PSC with the structure glass/FTO/CH₃NH₃PbI₃₋ₓClₓ/Spiro-OMeTAD/Ag. From the analysis above, it was...
Table 2: The defect parameters for the Gaussian distribution.

|                | FTO          | TiO₂         | CH₃NH₃PbI₃₋ₓClₓ | Spiro-OMeTAD |
|----------------|--------------|--------------|-----------------|--------------|
| Type           | Neutral      | Neutral      | Neutral         | Neutral      |
| Density defects (cm⁻³) | 1 x 10¹⁵     | 1 x 10¹⁵     | 2.5 x 10¹³      | 1 x 10¹⁵     |
| Electron capture cross-section (σₑ) | 1 x 10¹⁵     | 1 x 10¹⁵     | 1 x 10¹⁵        | 1 x 10¹⁵     |
| Hole capture cross-section (σₚ)    | 1 x 10¹⁵     | 1 x 10¹⁵     | 1 x 10¹⁵        | 1 x 10¹⁵     |
| Energy (eV)    | Above Eᵥ    | Above Eᵥ     | Above Eᵥ        | Above Eᵥ     |

Figure 3: (a) Open-circuit and current density (b) fill factor and efficiency as functions of FTO thickness for constant TiO₂ and CH₃NH₃PbI₃₋ₓClₓ thicknesses.

Figure 4: (a) Open-circuit and current density (b) fill factor and efficiency as functions of TiO₂ thickness for constant FTO and CH₃NH₃PbI₃₋ₓClₓ thicknesses.
observed that 100 nm, 50 nm, and 350 nm layer thicknesses for FTO, TiO$_2$, and CH$_3$NH$_3$PbI$_{3-x}$Cl$_x$, respectively, gave a better cell performance. Therefore, with these layer thicknesses, the J-V characteristics curve of the solar cell was computed and the result is as shown in Figure 6. From the J-V computation, a higher efficiency of 29.56% was attained which is an improvement from the one already reported value [10]. Also, a high open-circuit voltage of 1.45 V is achieved which is also an improvement of an experimental value (1.25 V) already reported [29]. Furthermore, the FF of 78.87% was attained. The high value implies better absorption of solar radiations in the absorber material.
3. Conclusion

In this work, the perovskite solar cell with the structure glass/FTO/ TiO₂/ CH₃NH₃PbI₃-xClₓ/Spiro-OMeTAD/Ag was successively simulated using SCAPS-1D software. FTO, TiO₂, and CH₃NH₃PbI₃-xClₓ thicknesses were varied to investigate their influence on the device performance. The simulation revealed that the variation of TiO₂ thickness has no significance change in the device performance, and an absorber thickness from 300 nm to 400 nm is suitable for better device performance and hence thicker absorber may have no much advantages. The simulation results further revealed that 100 nm, 50 nm, and 300 nm layer thicknesses for FTO, TiO₂, and CH₃NH₃PbI₃-xClₓ, respectively, gave a better cell performance as compared to 200 nm, 50 nm, and 600 nm layer thicknesses for FTO, TiO₂, and CH₃NH₃PbI₃-xClₓ reported in the literature.

Data Availability

The [layer parameters used in simulation] data used to support the findings of this study are included in the article.

Conflicts of Interest

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

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