Optimization of active layers thickness of perovskite solar cell: gpvdm simulation study

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Abstract

Optimization of individual layer/s thickness in any functional photoelectric device like solar cells is one of the most important design parameters. Experimentalists do have their own limitations in realizing extremely thin functional devices. However, layer thickness is such a crucial factor which helps in deciding overall power conversion efficiency of modern photoelectric and optoelectronic devices. In this device simulation study, thickness of different active layers in a typical perovskite solar cell (PSC) has been tuned to trace the optimal performance as energy conversion device. In the present work, a typical PSCs was constructed of poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS), perovskite and zinc oxide (ZnO) active layers. In addition to the active layers, suitable front and back metal contacts are taken into the consideration in the form of ITO and Al, respectively. The effect of net photon absorption and further utilization in successive active layers and junctions was the main point of exploration in the simulation. Through this analytical study, experimentalists will get benefitted in designing/implementing their resources towards advancement of PSC research.

Keywords: Perovskite, PEDOT:PSS, ZnO, Generation rate, Efficiency.

1. Introduction

Device level simulation of various functional photoelectric devices is one of the trending fields of research in recent years. Since few decades, computational physicists have provided an ample amount of theoretical suggestions and future strategies to the wide research community. Among all photoelectric devices, solar cells have gained much attention due to high energy demand and green route for energy generation. Different solar photovoltaic technologies like crystalline silicon (Si), a-Si, CdTe, CIGS, dye sensitized solar cell (DSSC), organic solar cells (OSC) [1, 2, 3], polymer solar cells [4, 5], perovskite solar cells (PSC) [6, 7] and generic solar cells [8, 9, 10] have been explored both, theoretically and experimentally. Recently, perovskite based solar cells have shown tremendous potential and hence advancement in the realization of high efficient solar energy conversion devices. However, in spite of being potentially viable technology, PSC is struggling a lot in large scale applications. Moderate to poor device stability and low transparency are few of the limiting factors behind leisurelier acceptance of PSCs. In our recent study, we have reported accounting of individual photon while they pass through the device either utilised or unutilised.

In the present work, we will mainly focus our selves in finding out the optimal layer thicknesses for the improved device performance. At the same time, the role of each junction will be also qualitatively discussed which would help in design and fabrication of modern ultrathin photoelectric devices.

2. Perovskite solar cell configuration

For the present simulation, a perovskite solar cell consisted of poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) as a hole transport layer (HTL) and zinc oxide (ZnO) as an electron transport layer (ETL) was adopted. PSCs under study are configured of three active layers and appropriate metal contacts for the collection of photogenerated charge carriers. Three different devices named PSC-1, PSC-2 and PSC-3 have been studied for the comparative current-voltage (IV) analysis based on device simulations under standard test conditions.

3. Device simulation

Each of the configurations of PSC was individually simulated with the help of gpvdm software to collect their performance as solar cell. To do that away, an AM 1.5 G light source was used for recording IV spectra of the PSCs. Applied voltage range was restricted between 0 and 1 V to get the quantitative information about the photogenerated carriers which ultimately resulted in photocurrent. Optimal and suggestive parasitic resistances were choosen by default with the help of electrical simulation tool. Resulted output in the form of IV response and images have been recorded and presented to compare the power conversion efficiencies (PCE) of PSC-1, PSC-2 and PSC-3.

4. Results and discussion

At a very first instance, it is worth remembering that the overall power conversion efficiency of any solar cell would be at the highest precedence while optimizing the rest of the criteria. Hence, we have straight away focused ourselves to look into the IV curves of all three PSCs and are presented in Fig-1 for comparison purpose. As one can notice that, all of the configurations possessed very high open circuit voltage (V_{oc}) more than 0.85 V. In addition, eye catching square IV curves assured high fill factor due to selectively chosen parasitic resistances. However, there is a significant difference in the photocurrent values under short circuit condition. PSC-1 lagged behind by almost 15 A/m^2 while compared with the others. It is worth citing Table-1 for referring the thickness values of the active layers in all PSCs. It is interesting to observe that PSC-1 utilized highest thickness of all the layers and still struggled while working as solar cell. The eye catching observation leads us to explore further about individual junctions in the device which might had play a role underneath. Before going into further detailed discussion, let us just revisit the Fig-1 (also Table-1) to acknowledge very high short circuit current for rest of the devices. It highlights the importance of selection of active layer thickness and needs much attention. To do so, we have gathered spectral distribution of photogenerated carrier as available photons travel down different active layers and junctions. As it can be seen from Fig-2 (a), (b) and (c), PEDOT:PSS layer get exposed to incident AM 1.5 G source and available photons start travelling under the effect of natural band bending and the applied potential (while recording the IV). It is believed that both, absorption and photo conversion solely depends on the material aspects and not on their interface/s. As in our previous report, spectral profiles of successfully absorbed photons in devices PSC-1, PSC-2 and PSC-3 would guide in providing pathway for analysing the depth profiling of effective photo-generated carriers. Hence, it is worth mentioning again here in that the number density of available photons

which is being passed though the layer can be influenced by (1) absorbed photons in all previous/same layer/s, (2) successful conversion of photons into the free carriers in all previous layers and (3) reflected photons from the ITO surface. As previously understood and reported, the number of photons get decreased sharply at PEDOT:PSS/Pervoskite interface showing high rate of conversion of photons into photogenerated carriers (electrons and holes). Noteworthy, PEDOT:PSS which was believed to be HTL only, also take part in absorbing selective energy photons. It was very interesting to note that photons also get utilized at ZnO/Al interface and produce photogenerated electron-hole pairs contributing in the photocurrent. Considering all this analytical observations derived based on device level simulation study, one can notice that excess thickness of even an active layer hinders the efficient utilization of each photon and overall PCE. Detailed analysis of photo conversion from each of the junctions in a typical device may lead us to find most suitable PSC configuration facilitating maximum power conversion at low material cost.

5. Conclusion

In conclusion, through the present analytical simulation study, the role of individual layer thickness on overall photoabsorption and charge carrier generation was understood. Effect of such layers on short circuit current was scrutinized to optimize the device efficiency from 3.05% to 3.98%. Profiles of photogenerated carriers in different layers provide a pathway to design perovskite based solar cells. Such theoretical study will enlighten a pathway for research community to design and fabricate highly efficient nanojunction optoelectronic devices.

Acknowledgement

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Table 1 Solar cell parameters extracted from simulations of PSCs utilizing different layer thicknesses.

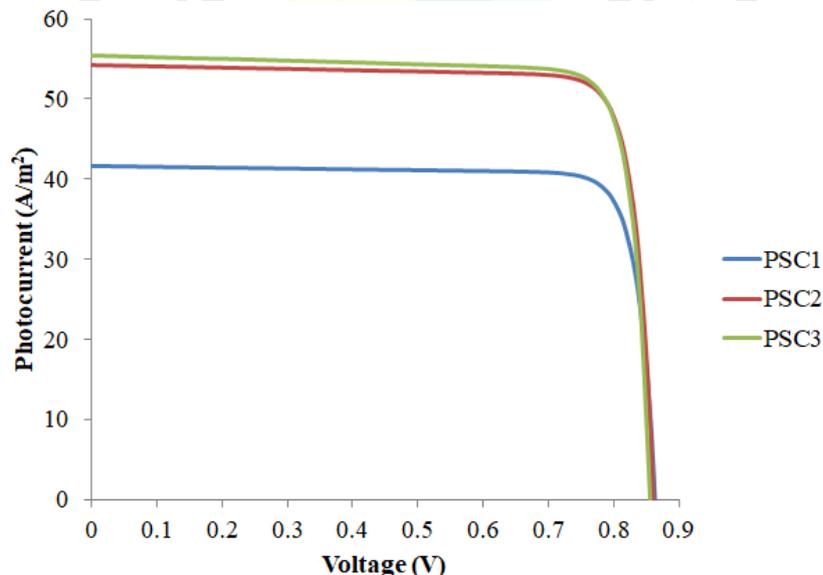| Parameter	PSC-1	PSC-2	PSC-3
Device thickness (nm)	1025	625	375
V_{oc} (V)	0.862	0.86	0.855
J_{sc} (A/m^2)	41.62	54.22	55
FF (%)	85	84.54	84
η (%)	3.05	3.94	3.98

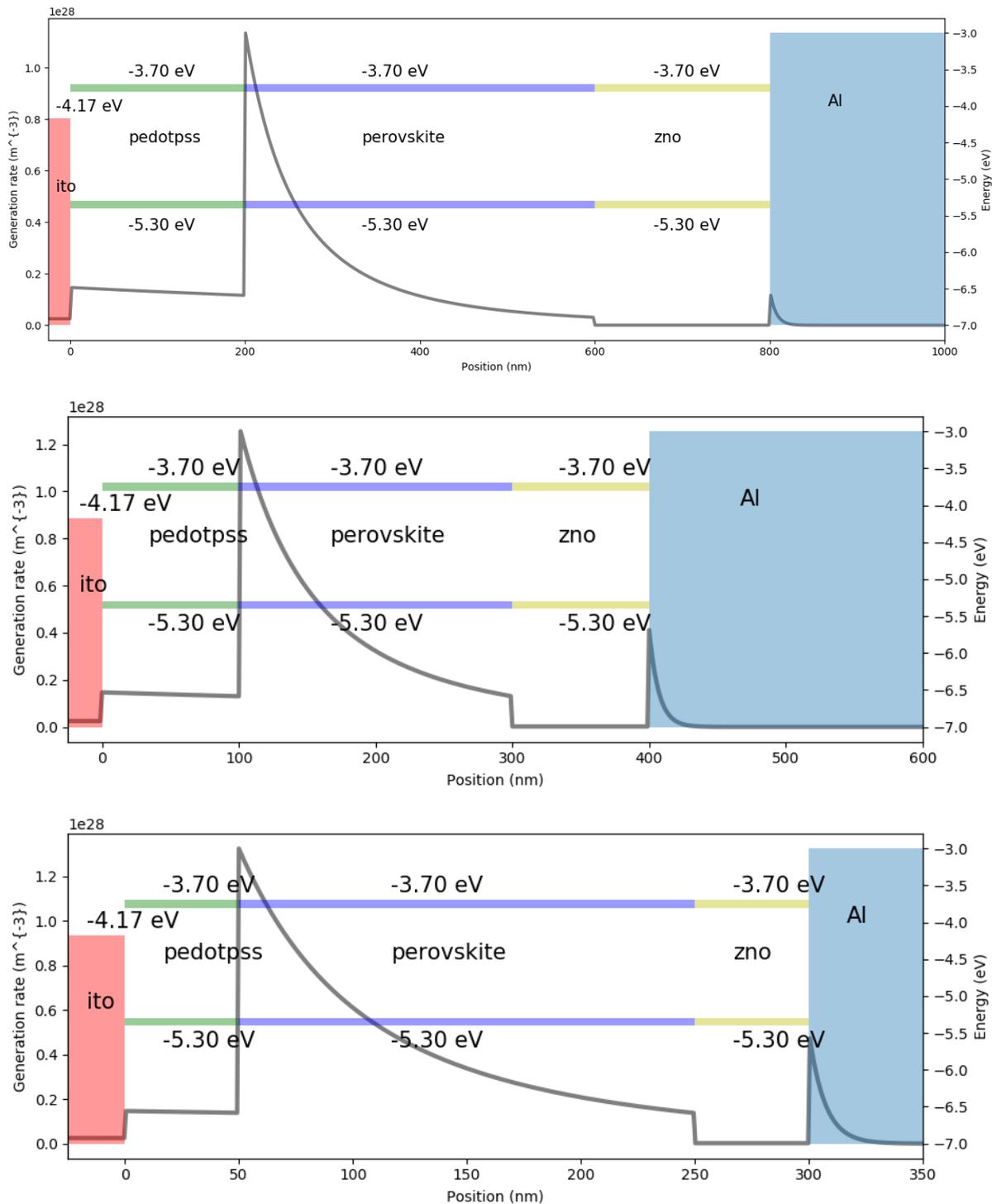**Figure 1 IV characteristic curves of PSCs**

Figure-2: Generation rate profiles in individual layers of perovskite solar cells utilizing different thicknesses (a) 1025 nm, (b) 625 nm and (c) 375 nm.