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Investigation of highly efficient methyl ammonium lead halide perovskite solar cell with non-textured front surface

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ABSTRACT

High quality methyl ammonium lead iodide ($MAPbI_3$) perovskite material based single junction solar cell was investigated by simulation. We observed a systematic variation in device performance due to a variation in optical absorption of the active layer. By changing thickness of absorber layer from 50 nm to 1000 nm, we obtained power conversion efficiency (PCE) of the photovoltaic devices varying from 7.9% to 21.1%. Its open circuit voltage (V_{oc}) varied from 1.26 V to 1.16 V, short circuit current density (J_{sc}) varied from 7.56 mA/cm^2 to 22.61 mA/cm^2 while the fill factor (*FF*) remained constant at 83% in this variation. Front surface of the solar cell was kept non-textured, however, back reflection of unabsorbed light was used in the analysis. The maximum PCE of 21.1% and J_{sc} of 22.61 mA/cm^2 was observed for the solar cell with 1000 nm absorber layer. The J_{sc} and device efficiency increases with increased thickness of absorber layer (d_i). Therefore, higher PCE can be obtained with a thicker absorber layer. However, we identify that, with 94 nm thick absorber layer, the rate of change of PCE is equal to the rate of change of J_{sc}, due to the thickness variation. In this cell with 94 nm thick absorber layer (Cell-94), the PCE was 11.5%, nearly half of the PCE obtained with 1000 nm absorber layer. In the Cell-94, the diode ideality factor was 2.04, and reverse saturation current density was 6×10^{-13} Amp/cm^2.

1. Introduction

Recent development in methyl ammonium lead iodide ($MAPbI_3$) perovskite material has drawn intense interest to explore its potential in fabricating photovoltaic (PV) solar cell. Apart from the iodide [1–3] $MAPbI_3$, its chloride [4], bromide [5] and mixed halides [6] were also investigated. Among the various halide perovskites the iodide one shows attractive optical absorption [7], carrier mobility (500–800 cm^2 volt^{-1} s^{-1} [8]), diffusion length [9,10], high lifetime [11,12] that can be even more than 15 μs [13], photo sensitivity and device performance [14–16]. These perovskite materials have superior opto-electronic properties than thin film amorphous silicon semiconductors. A simple preparation technique [17–19], superior crystallinity [20,21] and optoelectronic properties are few of the attractive features that invited various research groups to explore the material for solar photovoltaics. A number of theoretical [22–25], experimental investigations [1–21,26,27] and review work [28–31] were also carried out to understand and explore its photovoltaic capabilities. It was reported that a careful preparation of material and device fabrication can lead to a larger crystallite grain size [20], lower defect density

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[32,33] and higher device efficiency [8]. Even though these materials are prepared in a simple technique, yet its defect density remains remarkably low.

However, this material is not free from its limitations. Degradation is one of the most important aspects of the device. It is thought that due to poor thermal conductivity of this material, the heat inside the perovskite material may create thermal stress [34], due to which ionic migration [33,34] within the bulk material leads to vacancy related defects [35]. In that respect a thinner perovskite layer may help in avoiding such a rapid degradation. Therefore, most of the experimental researches are limited to thinner perovskite layer. Ferro-electric hysteresis [36,37] is another effect that bring uncertainty to the experimental measurements. It was reported that a faster or slower scan rate [38], forward or reverse voltage scan [10,39], can change the current density- voltage (J-V) characteristic curve significantly, thereby the experimental error can mask the actual device characteristics. A standardized scan (0.01 V/sec [38]) or voltage sweep rate can reduce such an error. Furthermore, errors in experimental investigation is not very uncommon. For example, in reference [7], experimental results on open circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (*FF*) and power conversion efficiency (PCE) of perovskite solar cells shows variable measurement errors, as well as trend of variation is not very clear.

In order to systematically explore performance characteristics of such an organic-inorganic halide $MAPbI_3$ perovskite solar cell, we used numerical simulation, where the experimental errors are avoidable and a systematic device characteristics can be explored. We used a simple device structure, with indium tin oxide (ITO) as front electrode, TiO_2 as electron transporting layer (ETL), $MAPbI_3$ as photo-sensitive active layer, and Spiro-MeOTAD as hole transporting layer (HTL) [40,41] and gold (Au) as back electrode. Although ZnO can also be used as ETL [42]. Even though the energy levels of the valence and conduction bands of the materials depends upon preparation condition and may require additional buffer layers, yet we investigated the devices without such buffer layers. Although, it can be predicted theoretically that a thicker absorber layer can generate more electron-hole pairs, therefore increased J_{sc} and efficiency can be achieved, however, in practice, several other inter-dependant parameters may act against such a trend to mask the expected high efficiency. Therefore, simulation or theoretical results can be considered as experimentally achievable limiting values. In this article we report our investigation of structure of a perovskite solar cell where efficient photovoltaic conversion takes place.

2. Theoretical

Photovoltaic energy is generated after absorption of light in solar cell. The light absorption ($I(\lambda)$) in active layer of a solar cell creates energetic electron-hole pairs that should be separated before recombination. The light absorption, in a layer of thickness *d* and absorption coefficient α, follows Beer Lambert's exponential relation

$$I(\lambda) = I_0(\lambda)\left(1 - e^{-\alpha d}\right) \tag{1}$$

here $I_0(\lambda)$ is the spectral distribution of incident light, λ is wavelength. This means, a thicker layer and material of higher absorption coefficient can have higher optical absorption. Total light absorption can be expressed by integrating the Eq. (1). The integrated light absorption (Abs_1) and J_{sc} are known to be related as follows:

$$J_{sc} = A_1 q \int_{\lambda 1}^{\lambda 2} I(\lambda)\, d\lambda = A_1 q Abs_1 \tag{2}$$

Here A_1 is a constant related to external quantum efficiency (EQE), $I(\lambda)$ is spectral distribution of absorbed light, the integration range (λ1, λ2) is the wavelength range that dominantly contribute to J_{sc} or photovoltaic energy generation. Here

$$Abs_1 = \int_{\lambda 1}^{\lambda 2} I(\lambda)\, d\lambda \tag{3}$$

The photo-generated carriers are separated by the ETL and HTL layers. However, all these carriers cannot be collected, as some of them are lost by Shockley-Read-Hall type defect mediated recombination ($E_{L(SRH)}$), Auger recombination (E_{Auger}) and band to band recombination (E_{BB}). This carrier separation and recombination in a PV device depends on various factors like thickness and opto-electronic properties of the materials. In addition to the electronic loss, optical loss ($E_{L(opt)}$) also plays a significant role in device performance. It depends upon optical design of the device, for example, introducing texturing at the front surface will reduce reflection loss of incident light, therefore $E_{L(opt)}$ will become lower. Few of the major optical loss channels are, reflection at the front surface, parasitic absorption at the ETL, HTL layers, transmission loss of unabsorbed light. The $E_{L(opt)}$ can significantly be reduced by using light trapping structure, in which reflection at the front surface is reduced and the transmitted light are reflected back to solar cell for further absorption. If E_{in} is energy of incident light and E_{out} is output electrical energy from a PV device and E_{Loss} is sum of other possible loss mechanisms, then cell output electrical energy can approximately be expressed as:

$$E_{out} = E_{in} - E_{L(opt)} - E_{L(SRH)} - E_{Auger} - E_{BB} - E_{Loss} \tag{4}$$

This expression (4) indicates that any kind of loss mechanism can degrade output power from the device. Here E_{in} is constant incident light, $E_{L(opt)}$ is another constant, however, the recombination losses can vary, as discussed later. The Fig. 1