Performance Optimization of MASnI3-based Perovskite Solar Cells

Abstract. Solar cells of hybrid organic-inorganic perovskites have attracted researchers and scientists all over the world. Perovskite solar cells outperform conventional silicon solar cells by achieving higher conversion efficiency with a more stable performance. In this paper, a typical perovskite solar cell consists of 6 principal layers of materials: a protective glass layer, thin fluorine Doped Tin Oxide (FTO), Cd0.5 Zn0.5S as electron transportation layer (ETM), MASnI3 as perovskite active layer, CuSCN as hole transportation layer (HTM) and another gold (Au) electrode were utilized. This paper summarises the work that centred on the selective use of composite materials of the perovskite solar cell with a variation of the perovskite layer thickness. An optimization procedure is applied to increase the conversion efficiency and enhance the overall performance by varying the thickness and doping concentration of the main cell layers (i.e. ETM, absorber and HTM). The results showed that, by employing the optimum parameters, the conversion efficiency was increased from 12.86 to 26.68%.

Introduction

The silicon solar cell has so far been successfully reached an efficiency of 12 to 17.5 %, resulting in a comprehensive search for modern, more effective content. Thus, scientists who are working on hybrid photovoltaic materials started to investigate their efficiency extensively. Photovoltaic hybrids have opened the door for a new era by achieving better performance compared to inorganic silicon solar cells. Silicon was the main material used for manufacturing solar cells since the 1950s. Organic and inorganic hybrids have gained great attention by introducing perovskite solar cells since 2009 with efficiency starting from 3.8% to more than 23.3%. Perovskite solar cells have showed an extremely low cost, low complexity, and high performance parameters of the reference cell, listed in table 1. The performance parameters of the reference cell, taken from literature [10], and are listed in table 1. The structure of the proposed cell in the present work is planar perovskite solar cells with a structure of FTO/ Cd0.5Zn0.5S/ MASnI3/CuSCN, and another gold (Au) electrode.

Keywords: Modelling, Simulation, Perovskite Solar Cell, Photovoltaics, Inorganic Materials, Organic Materials.

Streszczenie. Ogniwa słoneczne z hybrydowego organiczno-nieorganicznego perowskitu przyciągają badaczy i naukowców na całym świecie. Ogniwa słoneczne Perowskitowe przewyższają konwencjonalne krzemowe ogniwa słoneczne, osiągając wyższą wydajność konwersji przy bardziej stabilnej wydajności. W tym artykule typowe perowskowe ogniwo słoneczne składa się z 6 głównych warstw materiałów: ochronnej warstwy szklanej, cienkiej domieszkowanej fluorem tlenku cyny (FTO), Cd0.5 Zn0.5S jako warstwy transportu elektronów (ETM), MASnI3 jako warstwy aktywnej perowskitu , zastosowano CuSCN jako warstwę transportującą dzury (HTM) i inną zlotą (Au) elektrody. Ten artykuł podsumowuje prace, które koncentrowały się na selektywnym wykorzystaniu kompozytowych perowskowych ogniwa słonecznego ze zmianą grubości warstwy perowskitu. Stosowana jest procedura optymalizacji w celu zwiększenia wydajności konwersji i poprawy ogólnej wydajności poprzez zmianę grubości i stężenia domieszki głównych warstw komórek (tj. ETM, absorbera i HTM). Wyniki wykazały, że przy zastosowaniu optymalnych parametrów wydajności konwersji wzrosła z 12,86 do 26,68%. (Optymalizacja wydajności ogniw słonecznych perowskowych opartych na MASnI3)

Keywords: Modelling, Simulation, Perovskite Solar Cell, Photovoltaics, Inorganic Materials, Organic Materials.

Słowa kluczowe: ogniwa fotowoltaiczne Perowskitowe, optymalizacja

Stress. The perovskite makes a promising candidate in this comparison. The main aim of the design of a highly efficient solar cell is to maximize the effective energy conversion (PCE) ratio to cost. And due to this rapid investigation and enhancement of the perovskite band, around 2013-2018, an efficiency of 15.7% to 22.7% were reported in the literature [6-7]. Among various perovskite materials such as MAPbBr3, MAPbCl3, MAPbBr3, MASnI3 and MAPbI3, it is observed that MASnI3 iodide is a good candidate due to its excellent electrical and optical properties, low-temperature solubility, long-life, and ferroelectricity. With various design techniques not only for the absorber layer but also in all other six layers, the efficiency of perovskite solar cells can be further enhanced [8-9].

In this paper, a parametric study is performed on the planar perovskite solar cells with a structure of FTO/ Cd0.5Zn0.5S/ MASnI3/CuSCN to find the optimum layer thickness and doping concentration to increase the overall conversion efficiency.

Cell structure and input parameters

The structure of the proposed cell in the present work is based on a perovskite solar cell. As shown in figure (1), the structure consists of four layers, Cd0.5 Zn0.5 S as ETL layer, MASnI3 as the absorber layer, CuSCN as HTL layer, and fluorne-doped tin oxide (FTO) as the transparent conducting oxide. The input parameters of the reference cell were taken from literature [10], and are listed in table 1. The structure was studied under the STC which is at a room temperature of 300 K, and 1000 W/m² irradiance levels.

The performance parameters of the reference cell, which are represented by JSC, VOC, FF, and efficiency, are calculated based on the basic parameters of the materials. The major parameters that have a direct impact on the cell performance are the doping density, the thickness, and the defect density of the layers. SCAPS simulation software is employed to perform all the necessary calculations [10].

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Table 1. Input parameters of the reference cell taken from Ref. [10].

<table>
<thead>
<tr>
<th>Parameters</th>
<th>FTO</th>
<th>Cd0.5Zn0.5S</th>
<th>MASnI3</th>
<th>CuSCN</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thickness (µm)</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>Eg (eV)</td>
<td>3.5</td>
<td>2.8</td>
<td>1.3</td>
<td>3.4</td>
</tr>
<tr>
<td>χ (eV)</td>
<td>4</td>
<td>3.8</td>
<td>4.17</td>
<td>1.9</td>
</tr>
<tr>
<td>εr</td>
<td>9</td>
<td>10</td>
<td>8.2</td>
<td>10</td>
</tr>
<tr>
<td>Nc (cm⁻³)</td>
<td>10¹⁰</td>
<td>10⁴⁴</td>
<td>10¹⁰</td>
<td>1.7 × 10¹⁵</td>
</tr>
<tr>
<td>µc (cm²/Vs)</td>
<td>100</td>
<td>100</td>
<td>1.6</td>
<td>0.0001</td>
</tr>
<tr>
<td>Na (cm⁻³)</td>
<td>10¹⁸</td>
<td>10¹⁸</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Nd (cm⁻³)</td>
<td>10¹⁵</td>
<td>10¹⁵</td>
<td>10¹⁵</td>
<td>10¹⁵</td>
</tr>
</tbody>
</table>

b. MASnI3 layer

On the other hand, the curves in figure (4) show a similar trend, as the absorber layer thickness increases, the Voc, Jsc, and PCE elevate while the FF was decreasing from 75.56 to 64.13 %. The increment in the Jsc was due to the high absorption of photons by this layer [10]. As a result, the elevation of the excess carrier concentration causes the Jsc to increase and consequently the efficiency. The optimum values of the doping density, as well as the thickness for this layer, are 10¹⁵ cm⁻³ and 1 µm, respectively, which leads to a maximum PCE of more than 20 %.

Fig. 4. The impact of the MasSnI3 layer thickness on the cell parameters.

The defect density variation has no noticeable influence in this layer, as Nt changing from 10¹⁴ to 10¹⁷ cm⁻³ there is no change in the output parameters of the cell and the efficiency was constant at 20.87 %.

c. Cd0.5 Zn0.5 S layer:

After having the optimum values of the thickness and doping density in the previous layer, the next step is to study the impact of the input parameters variation in this layer on the cell performance.

The thickness of this layer has a significant effect on the performance, as the thickness increases from 0.2 to 1 µm, the open-circuit voltage is almost constant at 1.2 V while the short circuit current elevates excessively from 5.308 to 22.658 mA/cm² and this is because thick layer in restricted range leads to higher absorption, and thus higher photo-generated carriers and higher Jsc, which finally leads to an increment in the efficiency [12] [13]. Figure (5) shows the aforementioned impact of layer thickness.

Increasing the doping density Nd has a trivial impact on the performance of the cell, where the Voc, as well as the PCE, starts to degrade gradually while the Jsc increases slightly due to the increment in the carrier concentration. Thus, the optimum Nd for this layer is 10¹⁵ cm⁻³ that gives the highest PCE.
d. D.TO layer:
Any solar cell with good design and high performance must have a thin layer of anti-reflection material of a heavily doped n-type material, which is in this work a layer of FTO. This layer will be a window for the light and acts as an anti-reflecting layer, which reduces the reflection losses at the same time; and this is the reason behind the advantage of using TCO material in any design. The effect of the doping and the thickness of this layer can be neglected as it will not contribute to the absorption and as a consequence in the generation of charge carriers.

Optimum cell parameters
The perovskite solar cell that has the best performance in this work is a cell that gives a PCE of 26.68%, open-circuit voltage of 1.628 V, short circuit current of 22.682 mA/cm², and fill factor of 72.21%. It has input parameters for the thickness and doping density as illustrated in table 2.

The energy band structure, as well as the quantum efficiency response of the optimum cell, are shown in figures (6) and (7).

Table 2. Input parameters of the optimum structure.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Doping density (cm⁻³)</th>
<th>Thickness (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CuSCN</td>
<td>10¹⁰</td>
<td>0.2</td>
</tr>
<tr>
<td>MA5Sn3</td>
<td>10¹⁰</td>
<td>1</td>
</tr>
<tr>
<td>Cd₀.₅Zn₀.₅S</td>
<td>10¹⁰</td>
<td>1</td>
</tr>
<tr>
<td>FTO</td>
<td>10¹⁰</td>
<td>1</td>
</tr>
</tbody>
</table>

Figure 6. Energy Band Structure of the optimum cell.

It can be observed from the band diagram of the perovskite layers (figure (6)) that the majority of photogenerated carriers are produced at the interface layers (HTM/Absorber and Absorber/ETM), thus, it is quite necessary to have these interfaces optimized and aligned properly in order to increase the open circuit voltage and hence the conversion efficiency. It also found that the optimum thickness of the Cd₀.₅Zn₀.₅S and MA5Sn3 was 1µm, whereas it was 0.2 µm for the CuSCN layer. On the other hand, it was observed by simulation results that the optimum doping concentration is 10¹⁹ cm⁻³ for the MA5Sn3 and CuSCN layers, but it is 10¹⁵ cm⁻³ for the Cd₀.₅Zn₀.₅S. Results demonstrate the promising future of perovskite solar cells by carefully tuning the most sensitive parameters that play a significant role in the overall performance of the cell such as the layer thickness and the doping concentration as proposed in this paper. More parameters can be explored in future works and their impact on the cell’s conversion efficiency can be investigated.

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