Optimization of Electrical Performance of Defected $n^+\text{-}p\text{-}p^+$ Solar Cell with CdS/BaSi$_2$/Cu$_2$O Heterostructure Using SCAPs 1D

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Research Article

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Abstract

Present study investigates the performance of BaSi$_2$ based BSF structure solar cell. SCAPS 1D simulator has been employed to investigate the heterostructure solar cell. To decrease the recombination loss due to minority carrier, a new configuration is proposed by inclusion of the p-type cuprous oxide (Cu$_2$O) as BSF layer. The Cu$_2$O BSF layer width varying in range 0.1 to 0.4 µm to analyze the feasibility of device for optimum performance. The anticipated structure consists of ZnO/CdS/BaSi$_2$/Cu$_2$O layers and offers the maximum efficiency of above 24%. Parameters for example open circuit voltage ($V_{oc}$), short-circuit current density ($J_{sc}$), fill factor (FF), conversion efficiency ($\eta$) and quantum efficiency (QE) of the device have been analyzed graphically. The optimized structure may have significant impact on future development of advanced photovoltaic devices.

1. Introduction

In the last decade, thin film photovoltaic technology gains the interest of researchers due to high efficiency above 20%. To convert sunlight energy into electricity effectively low cost and efficient solar cell is necessary. Currently, researchers are yet exploring for innovative kinds of solar cell in addition 1$^{st}$ generation (Silicon based) as well as 2$^{nd}$ generation (thin film based) solar cells. Barium Silicide (BaSi$_2$) is a optimistic material for highly efficient thin-film heterostructure solar cell [1]. With atomic number 56, a delicate alkaline earth metal is barium (Ba) having silvery-gray colour in its elemental form. For photovoltaic applications the most favorable and suitable material is BaSi$_2$ due to its high stability and band gap of about 1.1-1.35 eV [2]. A good absorber can be made up of BaSi$_2$ in solar cell. It can be used to formulate an optimistic low-cost heterojunction solar cell because of earth’s abundant Ba and Si. BaSi$_2$ has favorable optoelectronic characteristics like high absorption coefficient ($\alpha$) of about $3 \times 10^5$ cm$^{-1}$, hence, used as a commendable absorber material for heterojunction solar cell [3-5]. Other optimum electric properties are suitable indirect bandgap, [6-10], large value of diffusion length of 10 µm [10, 11], as well as lifetime of 14 µs. Additionally, the absorption coefficient of BaSi$_2$ is 30 [12] to 40 [7] times greater as compared to single crystalline-Silicon (c-Si). The absorption of photons begins at 1.3 eV and reaches to maximum value at 1.5 eV in case of BaSi$_2$ based solar cells. This range is much changed to a value of 1.3-1.7 eV [7, 13] for a 900 nm thick film. One more promising material as an BSF layer is cuprous oxide (Cu$_2$O) along with energy band gap of about 2.1 to 2.61 eV [14]. Cu$_2$O is an non-toxic, low-cost, easily available material and have high absorption coefficient [15]. Cu$_2$O material has several advantages, comprising high abundant, nontoxicity, low-cost, relatively simple formulation method with specific square planar synchronization of oxygen and copper [16]. Cu$_2$O is extensively developed as an effective layer in some types of heterostructures [17-19]. To enables the incoming photons of high energy to go through the buffer layer and reached to absorber layer cadmium sulfide (CdS) is used. The photons reach the absorber layer with minimum absorption loss due to CdS. The band gap of CdS is of about 2.4 eV [20] supports this process. Zinc oxide (ZnO) is another promising material having wide and direct bandgap of 3.34 eV which makes it suitable as an opto-electronic material because of its
exposure in the visible region [21]. Moreover, ZnO was certainly developed under 1D nanostructures [22] and considerably rich in nature [23].

In this paper we report a graphical representation of numerical simulation for ZnO/CdS/BaSi$_2$/Cu$_2$O BSF solar cell by using SCAPS 1D software. We calculate different factors on which device performance depends. We suggest incorporation of Cu$_2$O BSF layer in solar cells to enhance the performance of device.

2. Simulation And Model

The proposed device schematics and structure is demonstrated in Fig 1a. The solar cell configuration consists of an ARC (antirefection coating) of ZnO, CdS(n) as buffer, BaSi$_2$ (p) as an absorber layer and Cu$_2$O(p+) as BSF layer. SCAPS comprises of three major equations of semiconductors: free electron continuity equations and holes, Poisson's equation. Nearly the whole constraints can be classified in SCAPS for example bandgap, electron affinity, doping, mobility, effective density of states and thermal speed etc. AM 1.5G as well as AM1.5D and AM0 illumination spectrum are also obtainable. Configurations of band helps to establish the amount of current passing over the heterojunction [24]. Fig. 1b demonstrated the energy band gaps of recommended BSF cell. Data of energy band gap attained from the SCAPS, depicted in g 1b explaining the bandgap of all materials. The band bending can be easily recognized between the BaSi$_2$ and CdS junction instigated through dissimilar doping concentrations employed in this study. The different layer parameters used in the simulations shown in the Table 1.

3. Results And Discussion

The heterojunction solar cell consists of CdS, BaSi$_2$ and Cu$_2$O as buffer, absorber and BSF layers respectively under AM1.5 conditions were simulated. The width of BSF and absorber layers varies to examine the cell performance whereas the other factor remain same. The value of Jsc have been attained up to 35.5 mAcm$^{-2}$ with to 24.4 % efficiency based on our recommended structure.

3.1. Effect of width of absorber (BaSi$_2$) layer

The impact of change in the width of BaSi$_2$ layer on the device performance is demonstrated in table 2 and Fig. 2. The width of BSF were maintained as 0.2 µm, however, for both CdS and ZnO layers value of thickness is 0.1 µm. Excessive number of carriers are generated due to incident photons absorption in the BaSi$_2$ layer that is the extremely substantial part of solar cell. In this work we examine the effect of BaSi$_2$ layer width on the suggested heterojunction solar cell limitations with varying thickness of BaSi$_2$ layer up to 5 µm. Major device limitations such as Voc, Jsc and $\eta$ were depicted and simulated in fig. 2. The outcomes reveals that Jsc and FF rises as the BaSi$_2$ layer width increase. The main cause of this kind of trend is primarily ascribed to enhanced absorption of incident light due to wider absorber layer [25]. The
BaSi$_2$ layer has been absorbed significant amount of incident photons with the rise of width of layer which precedes to the increase in photo electrons. The increase in the possibility of SRH (Shockley-Read-Hall) recombination because of growth of BaSi$_2$ layer width leads to the decrease in $\eta$ and Voc. Though, the width of absorber layer is directly impacting the cost of material which is the major drawback of solar cell with thicker absorber layer [25]. Hence, we are setting up the layer width to augmented value of 5 µm in present work. 5 µm BaSi$_2$ layer width permits to provide the $\eta$ of about 24.3% and Voc of 0.82 V.

### 3.2. Effect of thickness of BSF (Cu$_2$O) layer

A large doping concentration plays an important role at rear side of cell, to prevent the carriers’ recombination due to metallic rear contact. As a result, a BSF (back surface field) film is establishes having larger doping concentration than absorber layer. A thin layer of Cu$_2$O is merged to BaSi$_2$ and act as BSF region. The impact of change in Cu$_2$O width on working of device is demonstrated in table 3 and Fig. 3. The BaSi$_2$ and CdS width is 5 and respectively even as Cu$_2$O width changing from to . It can be noticed from the results that as the change in Cu$_2$O layer width do not affect the cell parameters (Voc, Jsc, FF, $\eta$) significantly. At the Cu$_2$O/BaSi$_2$ interface, an electric field is created which behave as space charge region (potential barrier) for drift of minority carriers to back surface. A 0.2 µm thick BSF layer permits the Jsc of ~ 35.656 A/cm$^3$ as well as the efficiency of about 24.27%.

### 3.3. Effect of operating temperature

Operating temperature directly affects the stability of solar cell, as it is described in previous research that $V_{oc}$ changes with the change in operating temperature. Fig. 4 demonstrated that the temperature changes between 300 and 600 K on the way to examine the implementation of defected CdS/BaSi$_2$/Cu$_2$O thin film solar cell. As displayed in fig 4 (a) the $V_{oc}$ reduces due to rise in temperature. With the rise of operating temperature, bandgap of bandgap decreases which also leads to growth in leakage current. An insubstantial variation can be noticed in $J_{sc}$, though, $V_{oc}$ reduces constantly from 0.8 to 0.2V. The $\eta$ and FF are also demonstrating the analogous trend of decline from 85 to 45% and 24.5% to 2.3% respectively.

### 3.4. Effect of variation in the concentration of defect density

Solar cell performance parameters are directly affected by a significant factor known as defect density. Absorber layer plays a crucial role in generating the photo-electric current. Therefore, the carrier recombination increases due to increase in defect density which leads to the decrease in device efficiency. We change the defect density from $10^{12}$ cm$^{-3}$ to $10^{19}$ cm$^{-3}$ to study the impact of defect density on the performance of device. It is observed that the defect density influences the output of device in a substantial manner as demonstrated in fig. 5. One can be noticed from fig. 5 that the Jsc starts decreasing when defect density increases above $10^{16}$ cm$^{-3}$. However, the efficiency decreases continuously with increase in defect density from $10^{12}$ cm$^{-3}$ to $10^{19}$ cm$^{-3}$. The results are in good agreement with the previous studies [26]. The carrier recombination increases due increase in defect
density which in order decrease the diffusion length and carrier lifetime, hence, the overall performance of device decreases.

**Conclusion**

Present work has developed a graphical representation of performance thin film heterojunction solar cell having Cu$_2$O BSF layer. SCAPS 1D simulator has been employed to investigate the heterostructure solar cell. To decrease the recombination loss due to minority carrier, a new configuration is proposed by inclusion of the p-type cuprous oxide (Cu$_2$O) as BSF layer. The Cu$_2$O BSF layer width varying from 0.1 to 0.4 µm to analyze the feasibility of device for optimum performance. The anticipated structure consists of ZnO/CdS/BaSi$_2$/Cu$_2$O layers and offers the maximum efficiency of 24.4%. Parameters for example open circuit voltage ($V_{oc}$), short-circuit current density ($J_{sc}$), fill factor ($FF$), conversion efficiency ($\eta$) and quantum efficiency (QE) of the device have been analyzed graphically. The optimized structure may have significant impact on future development of advanced photovoltaic devices.

**Declarations**

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Tables

Due to technical limitations, table 1 is only available as a download in the Supplemental Files section.

Table 2: Solar cell performance with respect to absorber layer thickness.

| BaSi2 width (m) | V_{oc} (V) | J_{sc} (mA/cm²) | FF (%) | η (%) |
|-----------------|------------|----------------|--------|-------|
| 2.0             | 0.90297    | 35.41688       | 77.7178| 24.8544|
| 3.0             | 0.851797   | 35.51242       | 81.4396| 24.635 |
| 4.0             | 0.825595   | 35.54912       | 83.2621| 24.4367|
| 5.0             | 0.809652   | 35.5646        | 84.2874| 24.2705|

Table 3: Solar cell performance with respect to Cu2O BSF layer thickness.

| Cu2O-BSF width (m) | V_{oc} (V) | J_{sc} (mA/cm²) | FF (%) | η (%) |
|--------------------|------------|----------------|--------|-------|
| 0.1                | 0.8096     | 35.5619        | 84.2877| 24.2686|
| 0.2                | 0.8097     | 35.5619        | 84.2874| 24.2705|
| 0.3                | 0.8097     | 35.5671        | 84.2872| 24.2723|
| 0.4                | 0.8097     | 35.5694        | 84.2869| 24.2739|

Figures
Figure 1

Schematic structure of Cu₂O BSF cell.

Figure 2

Solar cell performance with respect to absorber layer thickness.
Figure 3

Solar cell performance with respect to Cu$_2$O BSF layer thickness.

Figure 4

Solar cell performance with respect to operating temperature.
Figure 5

Solar cell performance with respect to defect density.

Supplementary Files

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- Table1.jpg