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Numerical Analysis on Design of High Performance CSTZ Solar Cells

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Abstract: The surging of photovoltaics has witnessed the boost of numerous fascinating approaches to the enhancement of power conversion efficiencies (PCE) of the devices. For the search of new metal-halide CZTS solar cell materials, tolerance factors are calculated from the ionic radius of each site and are often utilized as the critical factors to expect the materials forming CZTS structure. Significant progress in photovoltaic conversion of solar energy can be achieved by new technological approaches that will improve the efficiency of solar cells and make them appropriate for mass production. The paper presents the numerical analysis on design of high performance CSTZ solar cells with the help of MATLAB programming. The performance reliance on physical properties is estimated, together with the layer thickness, carrier density, defect density and interface defect density. The best possible the layer thickness and carrier density were originated in this study. The defect density in the absorber would be controlled for reducing the recombination. The interface between the layer of absorber and the layer of buffer is essential for the performance of that solar cell. The interface defect density is embarrassed to accomplish enviable conversion efficiency. The results confirm that the experimental works could be met with the theoretical analysis in this paper.

Keywords: Numerical Analysis, High Performance, CSTZ, Solar Cells, MATLAB

1. Introduction

Solar cells convert solar energy, in the form of electromagnetic radiation, into electrical energy. A standard solar cell is shown schematically in Figure ure. Sunlight is incident on the surface covered by a metallic grid acting as an electrical contact [1-4]. Between the grid lines photons are absorbed in a semiconductor which is covered by an anti-reflective coating to reduce reflection. Photons with energies larger than the band gap EG of the semiconductor excite electrons from the valence band to the conduction band, resulting in free charge carriers; electrons and holes. The charge carriers are separated by either a gradient in the charge carrier density or an electric field. In Figure ure, the charge carriers are separated by the electric field across the p-n junction and the electrons are transported through a load in the external circuit where they do work [1-6].

There is a wide range of other semiconductor material capable of producing solar cells of acceptable efficiencies. Both solid and liquid materials are used in solar cells. Homojunction, heterojunction, metal-semiconductor, and some dye-sensitized solar cells use all-solid structures, whereas liquid-semiconductor and many dye- sensitized cells use solid – liquid structures. These materials can be inorganic or organic. The solids can be crystalline, polycrystalline, or amorphous. The liquids are usually electrolytes. The solids can be metals, semiconductors, insulators, and solid electrolytes [7-13].

Recently, the high performance solar cell fabrication is a vital role in semiconductor optoelectronic devices design. Cu_2ZnSnS_4 (CZTS) is a talented material for the low-cost thin-film solar cells owing to it's the best direct band gap energy of 1.5eV and huge absorption coefficient of 10^4 cm^{-1}. The peak conversion efficiency for pure Cu_2ZnSnS_4 (CZTS) solar cells has been described with 8.4% [14]. In order to get the improvement of the conversion efficiency incessantly, complete analysis of the device operation apparatus is essential. The semiconductor Poisson equation and continuity relations of electrons and holes are realized by using iterative solution [15-19].

The rest of the paper is organized as follows. Section mentions the model and physical parameters of CZTS solar cell structure. Section III presents the mathematical modelling of the proposed solar cell structure. Section IV highlights the analysis on device system. Section V discusses on the simulation results and discussions those results. Section VI concludes the current workdone.

2. Model and Physical Parameters of CZTS Solar Cell Structure

The model structure of the CZTS solar cell appraised in this study is revealed in Figure 1. The model of back contact/CZTS layer/buffer layer/i-ZnO/ZnO:Al/front contact systems as a source for modelling CZTS solar cells. The alternative buffer layer to replace specific materials would be considered in the prospect study. The layer properties are mentioned based on CZTS layer/buffer layer/i-ZnO/ZnO:Al system. The values of layer thickness (W) for CZTS layer/buffer layer/i-ZnO/ZnO:Al are 600,100,80 and 450 nm, respectively. The values of relative permittivity ($\varepsilon/\varepsilon_0$) are 10,10,9, and 9, correspondingly. The values of mobility of electrons (μ_n) are 5, 100, 100, and 100 cm^2Vs, respectively. The values of mobility of holes (μ_p) are 1, 25, 25, and 25 cm^2Vs, correspondingly. The values of holes density (N_A) are 1×10^{16}, 0, 0, and 0 cm^{-3}, respectively. The values of electrons density (N_D) are 0, 1×10^{17}, 1×10^{17} and 1×10^{18} cm^{-3}, correspondingly. The values of band gap energy (E_g) are 1.45, 2.4, 3.3, and 3.3, respectively. The values of conduction band effective density of states (N_C) are 2.2×10^{18}, 2.2×10^{18}, 2.2×10^{18} and 2.2×10^{18} cm^{-3}, correspondingly. The values of valence band effective density of states (N_V) are 1.8×10^{19}, 1.8×10^{19}, 1.8×10^{19} and 1.8×10^{19} cm^{-3}, respectively. The values of Gaussian defect density (N_G) are 1.8×10^{13} (Donor), 1.8×10^{17} (Acceptor), 1.8×10^{16} (Acceptor) and 1.8×10^{16} (Acceptor) cm^{-3}, respectively.

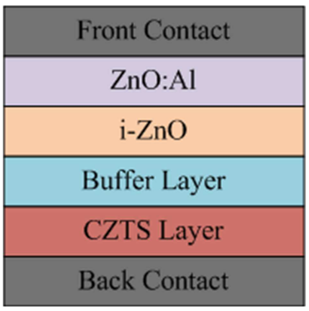

Figure 1. *Model Structure of CZTS Solar Cell.*

3. Mathematical Modelling

The hypothetical modelling is completed in the subsequent order. For short circuit current we know,

$$I_{\text{short circuit}}=I_0\left(\exp\left(\frac{qV}{kT}\right)-1\right) \tag{1}$$

where $I_{\text{short circuit}}$ is the short circuit current, I_0 is the diode saturation current, q is electron charge, k is the Boltzman constant, T is the temperature, and V is the voltage.

$$V_{\text{open circuit}}\approx\frac{kT}{q}\ln\left(\frac{I_{\text{short circuit}}}{I_0}\right) \tag{2}$$

where $V_{\text{open circuit}}$ is the open circuit voltage and others are as settled above.

Maximum output voltage,

$$V_m=V_{\text{open circuit}}-\frac{kT}{q}\ln\left(1+\frac{q}{kT}V_m\right) \tag{3}$$

Where all the parameters as settled above.

For ideal case scenario,

$$V_m=1,\ \frac{kT}{q}=0.026V \tag{4}$$

$$V_m=V_{\text{open circuit}}-0.026\ln\left(1+\frac{1}{0.026}\right) \tag{5}$$

$$V_m\approx V_{\text{open circuit}}-0.096 \tag{6}$$

Maximum output current,

$$I_m=-I_{\text{short circuit}}\left(1-\left(\frac{kT}{V_m}\right)\right) \tag{7}$$

Fill factor/ideality of the cell,

$$FF=\frac{V_mI_m}{V_{\text{open circuit}}I_{\text{short circuit}}} \tag{8}$$

Considering the best case where all the photon energy are improved into short circuit current, $I_m=I_{\text{short circuit}}$, fill factor becomes

$$FF\approx\frac{V_m}{V_{\text{open circuit}}} \tag{9}$$

$$FF\approx\frac{V_{\text{open circuit}}-\frac{kT}{q}\ln\left(1+\frac{q}{kT}\right)}{V_{\text{open circuit}}} \tag{10}$$

Considering an ideal case,

$$FF\approx\frac{V_{\text{open circuit}}-0.096}{V_{\text{open circuit}}} \tag{11}$$

$$FF\approx1-\frac{0.096}{V_{\text{open circuit}}} \tag{12}$$

This derived experimental equation will definitely assist to find the cells optimist from the imitation open circuit voltage result.

The conversion efficiency could be obtained from:

$$\eta=\left(\frac{V_mI_m}{P_{in}}\right)=\left(\frac{V_{\text{open circuit}}I_{\text{short circuit}}FF}{P_{in}}\right) \tag{13}$$

where, P_{in} is the solar radiation power incident on the unit area.

4. Analyzed the Device System

The study was accomplished to analyze the performance of CZTS solar cells based on the absorber thickness, carrier density, defect density and interface defect density.

4.1. Analysis on Absorber Thickness (CZTS Layer)

The absorber thickness of CZTS was most favourable to realize peak conversion efficiency. The peak conversion efficiency could be observed in the later section.

4.2. Analysis on Carrier Density in Absorber

The rising carrier density N_A can lessen lifetime for electrons and consequence in diminishing carrier collection prospect and current density for short circuit. The fewer carrier collection prospects can also depreciate the quantum efficiency of extended wavelength photons. Nevertheless the diminishing carrier density N_A enlarges the resistivity of the absorber and consequently condenses the involvement of holes current to current for short circuit. It is over and done with that a most favourable carrier density N_A exists for the major current for short circuit. Alternatively, the increasing carrier density N_A can diminish diode saturation current and augment open circuit voltage. The escalating voltage for open circuit can be described by the PN junction form:

$$V_{open\ circuit}=\frac{kT}{q}\ln\left(\frac{I_L}{I_0}-1\right) \quad (14)$$

$$I_0=qA\left(\frac{D_e n_i^2}{L_e N_A}+\frac{D_h n_i^2}{L_h N_D}\right) \quad (15)$$

It pursues a most favourable substrate carrier density will survive for maximum conversion efficiency. The result of carrier density N_A on the current density for short circuit, voltage for open circuit, fill factor and efficiency is evaluated.

4.3. Analysis on Defect Density in the Absorber

The SRH recombination was realized in the absorber of CZTS. The defect density based on fill factor could be evaluated with numerical analysis.

4.4. Analysis on Interface Defect Density Between the Absorber and the Buffer Layer

The interface properties between the absorber and the buffer layer are significant to realize the attractive efficiency of heterojunction solar cells. The interface defects of dislocations are affected by lattice mismatch between the two layers that appearance the interface. The performance weakening is owing to the rising interface recombination initiated by interface defects. Interface engineering is essential to be espoused to diminish interface recombination. One of the undertaking interface engineering expertises is to compliance the surface successfully prior to the deposition of the buffer layer.

5. Simulation Results and Discussions

The bandgap analysis for semiconductor solar cells based on silicon materials has been described. The material properties for solar cell have been demonstrated based on Absorption coefficient of silicon as the function of the wavelength and reflectivity. Finally, the characteristics of the silicon solar cell have been demonstrated to meet the high performance solar cell fabrication. According to the mathematical modelling of CZTS solar cell structure, there have been three analyses in this portion. Figure 2 shows the Fill Factor with respect to Open Circuit Voltage. Due to the increasing value of open circuit voltage, the fill factor would rise with respect to open circuit voltage. The fill factors were accepting to get the high performance of CZTS solar cell design. The defect density depends on the fill factor in real device fabrication. The recombination process could be affected based on the changes of fill factor in CZTS solar cell.

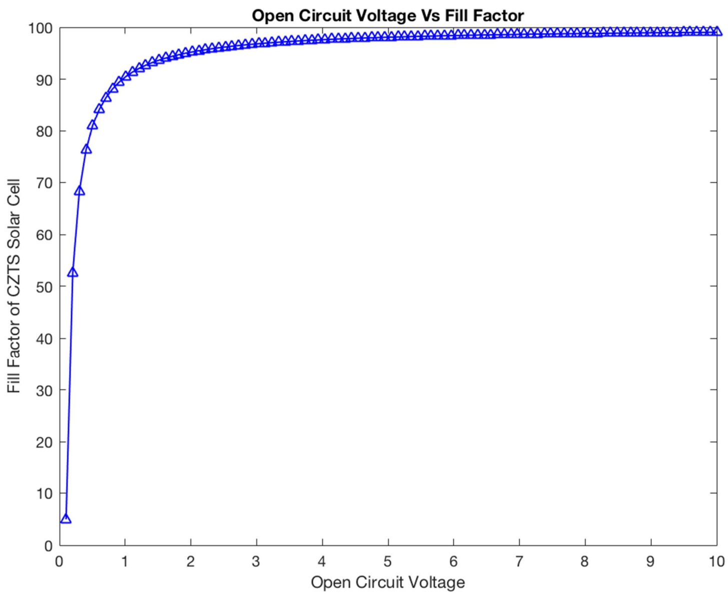

Figure 2. *Fill Factor with respect to Open Circuit Voltage.*

Figure 3 illustrates the Maximum Output Voltage with respect to Open Circuit Voltage. In this results, the observation of maximum output voltage were increased according to the incensement of open circuit voltages. The bound of defect density could be found in this section. Due to the changing of open circuit voltage, the maximum output voltage has to be altered because of the bound of defect density. The result says that the high performance CZTS solar cell could be formulated based on the relationship between open circuit voltage and maximum output voltage.

The high performance CZTS solar cell could be formulated based on the varying of physical parameters for real world condition.

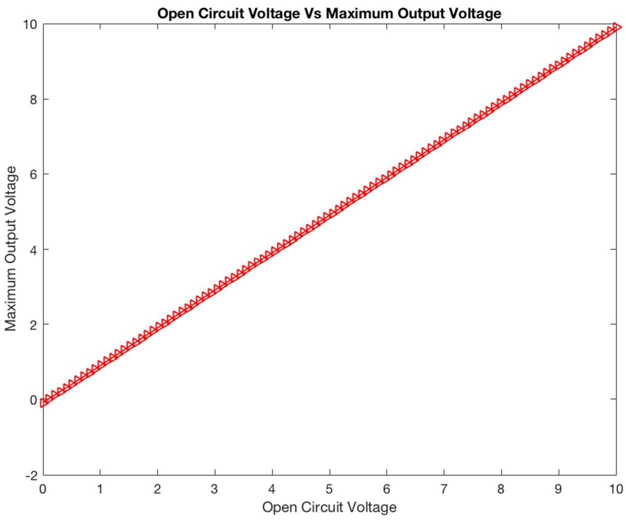

Figure 3. *Maximum Output Voltage with respect to Open Circuit Voltage.*

Figure 4 demonstrates the Short Circuit Current with respect to Open Circuit Voltage. The open circuit voltage of 10V with respect to short circuit current of 2.2 µA from these results could be observed.

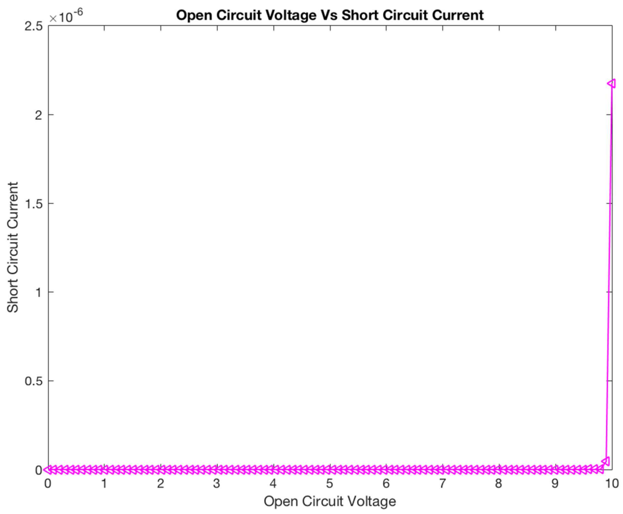

Figure 4. *Short Circuit Current with respect to Open Circuit Voltage.*

Figure 5 mentions the Conversion Efficiency with respect to Short Circuit Current. According to this analysis, the conversion efficiency directly proportion to short circuit current and the maximum value is at 2.2 µA of short circuit current in CZTS solar cell.

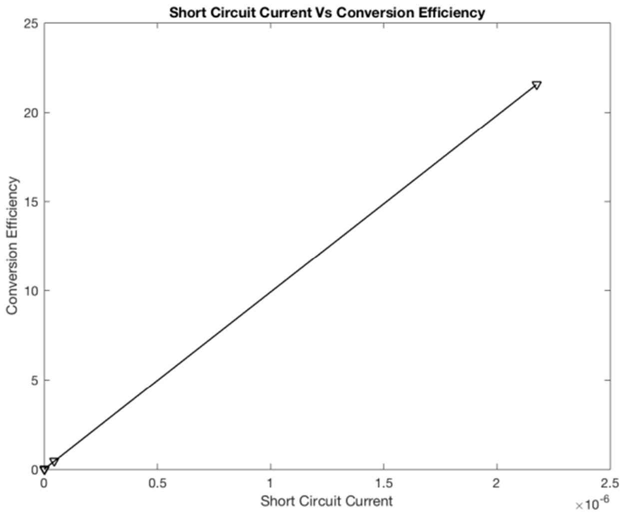

Figure 5. *Conversion Efficiency with respect to Short Circuit Current.*

6. Conclusions

The interface between the layer of absorber and the layer of buffer is essential for the performance of that solar cell. The interface defect density was embarrassed to accomplish enviable conversion efficiency. The results have confirmed the experimental works could be met with the theoretical analysis in this paper. The manipulation of properties of specific material on the performance condition of CZTS solar cells was scrutinized in the study. The complete modelling of solar cell device confirmed the most favourable layer thickness and carrier density of CZTS. The defect density in the absorber and the interface between the absorber and the buffer layer should be embarrassed to diminish recombination. The bound of defect density was originated in this analysis. The device modelling of high performance CZTS solar cells will be enhanced by extremely accepting the physical conditions of perceptible experimentation in the prospect study.

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