Numerical Simulation of Quantum Efficiency of Cd$_{0.8}$Zn$_{0.2}$S/CIGS Solar Cells

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Abstract: The paper presents a simulation study using the numerical simulator SCAPS-1D to model ZnO/Cd$_{0.8}$Zn$_{0.2}$S/CuIn$_{1-y}$Ga$_y$Se$_2$/CuInSe$_2$ structures. Effects of thickness of graded and ungraded CIGS absorbers and buffer layers on cell performance have been investigated with the aim to reach a higher efficiency. Quantum efficiency (QE) as function of wavelength and thickness of these layers was studied. The high efficiency of CIGS cells, in order of 22.05%, has reached with the absorbers thickness between 2 μm and 3.5 μm and with acceptor concentration of about $2 \times 10^{16}$ cm$^{-3}$. Other hand, we investigate the effect of Cd$_{0.8}$Zn$_{0.2}$S ternary compound buffer on the top of the p-CIGS cell. These simulation results give some important indication to enable further development of multilayer thin-film solar cells based on CuInGaSe$_2$ with Cd$_{0.8}$Zn$_{0.2}$S as buffer layer instead of CdS.

Keywords: Photovoltaic parameters, CIGS solar cells, CdZnS, SCAPS-1D, Modeling.

1. INTRODUCTION

A special quality of the Cu(In,Ga)Se$_2$ (CIGS) semiconductor is its variable band gap, which can be changed by varying the Ga/(In+Ga) ratio. When alloying the CuInSe$_2$ (CIS) with Ga to form CIGS thin films, the wider band-gap energy of the CIGS absorber layer can potentially better match the solar spectrum, and so increase the Voc parameter of cell with a little reduction of the short-circuit current density($J_{sc}$) [1, 2]. Conventionally CdS compound is serving as the buffer layer between CIGS and ZnO with band gap in order of 2.4 eV [3], which can be increased linearly by adding Zn to form Cd$_{1-x}$Zn$_x$S [4-7]. In this context, we have modeled the effect of varying the gap and the thickness of Cd$_{1-x}$Zn$_x$S buffer layer on the performance of CIGS solar cells.

On optimized buffer materials to replace the CdS buffer layer. The structure of our solar cells is: ZnO/Cd$_{0.8}$Zn$_{0.2}$S/CIGS/CIS.

In this paper, we reported the effect of layer thickness of CIGS graded and non-graded bandgap on the performances of this structure. The one-dimensional solar cell capacitance simulator (SCAPS-1D) is used to analyze numerically the performances of proposed cell.

2. NUMERICAL SIMULATION METHODOLOGY

2.1. Numerical model

In this present work, numerical modelling of multilayer CIGS thin film solar cell has been carried out by SCAPS-1D, version 3.2.01 computer software to investigate the effects on absorber band gap grading on the overall CIGS solar cell device performance. SCAPS-1D is one-dimensional computer software to simulate the AC and DC electrical characteristics of thin film heterojunction solar cells. It is developed especially for CdTe and CIGS solar cells at the University of Gent with LabWindows/CVI of National Instruments. SCAPS-1D simulator has been employed to model and analyze the solar cell as show in Figure 1.

![Figure 1: Diagram cell structure.](image)

2.2. Material Parameters

In this work we used the SCAPS-1D for simulation of solar cell performance. Quantum efficiency (QE) with the variation of thickness of CIGS absorber layers and Cd$_{0.8}$Zn$_{0.2}$S buffer layer. CdZnS alloy have a direct and
wide band gap energies ranging from 2.42 to 3.67 eV. For the simulation study, the depth profile is represented by an equivalent band-gap profile in the CdZnS buffer using the equation (1) proposed in [8], where the variable x composition of Zn in Cd(1-x)ZnxS

\[ E_g(x)[eV] = 2.42 + 0.9x + 0.3x^2 \quad (0 \leq x \leq 1) \quad (1) \]

The optical constants for the CIGS, CdZnS layers were calculated from the experimental data. The values of different material parameters used in this simulation are shown in Table 1.

### 3. SIMULATION RESULTS AND DISCUSSION

#### 3.1. Effect of Buffer Layer

**3.1.1. Effect of Cd_{(1-x)}Zn_xS Composition on Efficiency**

Figure 2 shows the efficiency \( \eta \) as function of the concentration \( x \) in Cd_{(1-x)}Zn_xS buffer layer in TCO/CdZnS/CIGS/CIS structure. As seen, for the lower addition of Zn we observe an increase of the efficiency of the cell which reached a maximum (21.5%) for \( x=0.2 \) corresponding to Cd_{0.8}Zn_{0.2}S compound. However, as \( x \) continued to increase we constate a progressive decline of efficiency. So, in the following of simulation study we use Cd_{0.8}Zn_{0.2}S as buffer layer instead of CdS.

**3.1.2. Effect on Internal Quantum Efficiency (IQE)**

Figure 3 illustrates the internal quantum efficiency (IQE) of ZnO/ Cd_{0.8}Zn_{0.2}S /CIGS/CIS structure with different Cd_{0.8}Zn_{0.2}S thicknesses in the range between 30 and 400 nm. The thickness of non-graded and graded CIGS layers are 3\( \mu \)m and 1\( \mu \)m with a doping density of \( N_A = 2 \times 10^{16} \) cm\(^{-3} \) and \( N_A = 5 \times 10^{16} \) cm\(^{-3} \), respectively. As we can see, the thickness of buffer layer has a significant impact on the IQE, particularly in short wavelengths region. As the junction is brought close to the surface, by reducing the Cd_{0.8}Zn_{0.2}S thickness, and since most of the short wavelength photons are absorbed in the vicinity of the surface, the collect efficiency of the cell is increased. Hence, the Cd_{0.8}Zn_{0.2}S film has to be as thin as possible.

#### 3.2. Effect of Absorber Layer

**3.2.1. Effect of Band Gap Energy of CIGS**

Figure 4 shows the efficiency of the ZnO/Cd_{0.8}Zn_{0.2}S(40nm)/CuIn_{1-y}Ga_ySe/CuInSe_2 solar cell as a function of band gap energy of CIGS non-graded. It is clear from the plot that an initial addition of Ga increased \( \eta \). However, as band gap energy
continued to increase, \( \eta \) soon reached a maximum and then started to decrease. When band gap energy of CIGS is equal to 1.32 eV, the solar cell performs better and, therefore, this value is considered to be optimum. Thus, the optimum efficiency of the proposed solar cell is \( \eta = 22.05 \% \).

3.2.2. IQE Study as Function of Absorber Layer Thickness

The thickness of CIGS non-graded and thickness of CIGS graded are found to be important parameters that directly influence the performance of solar cells, as shown in Figure 5 the quantum efficiency of the solar cell with variable absorber CIGS layer thickness. As mentioned earlier, when the p-type layer increases, more photons with longer wavelength can be collected in the absorber layer. This eventually will contribute to more electron-hole pair generation and collection as the longer wavelength photons can be absorbed [13]. The effect can clearly be observed in the quantum efficiency of the solar cell. The QE for a thicker absorber layer is much higher in the long wavelength portion as minority carrier diffusion length gains positively.

Next we analyze the effect of graded CIGS absorber thickness on the quantum efficiency of the ZnO/Cd\(_{0.8}\)Zn\(_{0.2}\)S/CIGS/CIS cell, as shown in Figure 6. The thickness of graded CIGS was increased from 400 nm up to 2400 nm. When the thickness of the graded CIGS is increased from 1600 up to 2400 nm, little effect on the QE is observed.

4. CONCLUSION

We reported the results of an analysis employing one dimensional simulation in order to optimize the performances of ZnO/ Cd\(_{0.8}\)Zn\(_{0.2}\)S/CIGS/CIS solar cell. We found that the p-layer and n-layer thickness strongly influence the performances of proposed solar cell. In the current work the performance improved with multilayer CIGS absorber when using the wider band gap Cd\(_{0.8}\)Zn\(_{0.2}\)S buffer layer in comparison to equivalent CdS/CIGS structures. Multilayer CIGS solar cell with a Cd\(_{0.8}\)Zn\(_{0.2}\)S buffer showed a highest efficiency of 22.05% with \( J_{sc} = 32.6 \) mA/cm\(^2\), \( V_{oc} = 0.880 \) V and Fill Factor = 76.7%.
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