

Optimization and improvement of a front graded bandgap CuInGaSe₂ solar cell

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ABSTRACT

This paper reports simulations of gradual bandgap CIGS absorber and its impact on the characteristics of a solar cell. The bandgap of the CIGS absorber varies linearly and drops from E_{gmax} (at the junction limit) to E_{gmin} (in the vicinity of the rear contact). We introduce an effective absorption coefficient based on this variation. We will demonstrate that this gradual profile contributes to an improvement up to 171 mV of the open circuit voltage V_{oc} of the cell that is linked to the modification of the internal electrical field distribution within the absorber. However, a joint reduction of 1.50 mA/cm² of short circuit current density, J_{sc} , is observed. Overall, the conversion efficiency increases from 19.2%, for a uniform bandgap absorber structure, to 24.9% in that case of gradual bandgap. Additionally, we investigate the impact of absorber thickness and temperature on cell characteristics.

1. Introduction

The quaternary chalcopyrite semiconductor alloy CuIn_{1-x}Ga_xSe₂, commonly noted CIGS, where x represents the ratio Ga/Ga + In, allows thin film solar cells to achieve high efficiency without the environmental concerns of CdTe. It exhibits a direct bandgap which is tunable from 1.02 eV to 1.68 eV [1–4] by adjusting x. Then, a high absorption coefficient can be achieved in a wide range of solar spectrum (400–1200 nm) [5,6]. The current record efficiency CIGS solar cell exceeds 21% [6–8] and is obtained for a bandgap energy of 1.15 eV for a material with x = 0.3. While the highest efficiency is theoretically expected to be obtained for a material bandgap of 1.4 eV (x = 0.7) which better matches the absorption of the solar spectrum, the experimental efficiency decreases when increasing the bandgap above 1.2 eV due to material fabrication issues. Improving the efficiency is then achieved using a bandgap grading within the absorber material. It consists on a spatial distribution of the x parameter [9]. This beneficial aspect of bandgap grading appeared first as a side effect of the three stage co-evaporation process and it was then used for optimizing cells performances [10–12]. Several profiles of gradual bandgap structures have been proposed and simulated. What we will hereby call "front grading" represents the gradual increase in Ga concentration from back contact toward the junction interface. It contributes to widen the material bandgap at the front contact allowing the increase of V_{oc} . So,

"back grading" would have consisted in the gradual decrease of the bandgap toward the back contact, then enhancing carrier collection and reducing recombination rate at the metallurgical contact. Double grading is the combination of those two approaches and is also characterized by the minimum bandgap location within the absorber material depth [10,13,14].

In this work, we focus on the front grading approach. It increases the value of the conduction band level near the CdS/CIGS junction leading to lower recombination level in the space charge region and to increase the open circuit voltage V_{oc} [15]. This study aims to use a simple model of such a gradual bandgap absorber in which the spatial distribution of material absorption that is linked to the variation of the bandgap is converted into a constant effective absorption coefficient all over the absorber depth. The linear gradual profile is then optimized to improve the cell performances. Finally, the behavior of such a gradual absorber structure under temperature fluctuations is investigated on V_{oc} and efficiency values.

2. Theoretical model

Optical absorption provides information about the band structure and the bandgap energy of semiconductor materials. The absorption coefficient of a uniform bandgap crystalline semiconductor layer in the high absorption region may be described by the model of Tauc et al.

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[16,17] given below.

$$\alpha = \begin{cases} 0 & \text{for } 0h\nu < E_g \\ \frac{A}{h\nu} (h\nu - E_g(x))^m & \text{for } h\nu > E_g \end{cases} \quad (1)$$

where A is a constant that depends upon the effective masses of both electrons and holes in the semiconductor, ν is the frequency of the incident radiation and m an index depending on the type of optical transitions caused by absorbed photons, $m = 1/2$ for direct transitions.

Fathipour et al. [18] shows that the absorption coefficient, α_{eff} , of a gradual bandgap material can be described the same way as for a uniform bandgap material using the following formulation:

$$\alpha_{\text{eff}} = \begin{cases} 0 & \text{for } 0 < h\nu < E_{g\min} \\ \frac{2}{3}\alpha_{\min} \left(\frac{h\nu - E_{g\min}}{E_{g\max} - E_{g\min}} \right) & \text{for } E_{g\min} < h\nu < \frac{3E_{g\max} - E_{g\min}}{2} \\ \alpha_{\min} & \text{for } \frac{3E_{g\max} - E_{g\min}}{2} < h\nu \end{cases} \quad (2)$$

Where $\alpha_{\min}$ is calculated by Eq. (1) for $E_g = E_{g\min}$. $E_{g\min}$ is the lowest bandgap value (near the back contact) and $E_{g\max}$ the highest bandgap (near the CdS/CIGS interface).

In this study we have assumed that the bandgap variation is due to the change in the conduction band level. The linear bandgap variation from $E_{g\max}$ to $E_{g\min}$ as function of position along the CIGS absorber depth is given by the following formula [18]:

$$E_g(x) = E_{g\max} - \beta x \quad (3)$$

$$\beta = \frac{(E_{g\max} - E_{g\min})}{d} = \frac{\Delta E_g}{d} \quad (4)$$

Where d is the thickness of the CIGS absorber layer. The bandgap energy profile is illustrated in the Fig. 1.

We used the Varshni relation to describe the temperature dependence of the bandgap energy [20]:

$$E_g(T) = E_g(0) - \frac{\alpha T^2}{\beta + T} \quad (5)$$

Where $E_g(0)$ is the bandgap value at $T = 0$ K, α and β are constants [21,22].

As compared to the uniform bandgap case, the bandgap variation ΔE_g (Eq. (4)) within the absorber modifies the electrical field distribution. It contributes to improve V_{oc} and the collection of generated electron-hole pairs as well as to reduce the bulk recombination. This electrical field modification can be expressed as [23].

$$\xi = \frac{d\Delta E_g}{dx} \quad (6)$$

The electron diffusion length is [9]:

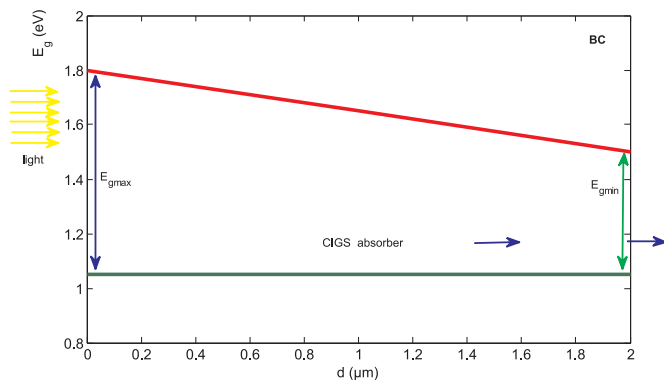


Fig. 1. Front bandgap energy profile of the CIGS absorber layer.

$$Ln_{\text{eff}} = \frac{ln}{\sqrt{1 + \left(\frac{\xi ln}{2V_T}\right)^2} - \frac{\xi ln}{2V_T}} \quad (7)$$

with V_T the thermal potential.

The dark saturation current density of a variable bandgap material can be approximated by [9]:

$$J_0 = J_{0\min} \left(\frac{2V_T}{\Delta V_g} \right) \quad (8)$$

$$\Delta V_g = \frac{\Delta E_g}{q} \quad (9)$$

Where $J_{0\min}$ is the dark current for a material with uniform bandgap energy $E_{g\min}$.

The open circuit voltage V_{oc} is expressed as [24]:

$$V_{OC} = \frac{nkT}{q} \ln \left(\frac{J_{ph}}{J_0} + 1 \right) \quad (10)$$

with q , the electron charge and n the diode ideality factor.

The total illumination current density in the case of the gradual bandgap is written as [19]:

$$J_{ph} = \int_{\lambda_{\min}}^{\lambda_{\max}} N_p (1-R) [1 - \exp(-\alpha_{\text{eff}} d)] d(h\nu) \quad (11)$$

Where N_p is the photon density of the incident light at the absorber surface and R the reflection coefficient.

3. Results and discussion

The open circuit voltage V_{oc} , the photo-generated current density J_{ph} , the fill factor FF and the efficiency of cells using gradual and uniform bandgap absorber material have been calculated and compared (all other parameters being identical). The maximum bandgap energy $E_{g\max}$ near the front interface as been varied from 1.15 to 1.6 eV. The minimum bandgap energy $E_{g\min}$ at the back contact was chosen to 1.15 eV. This value corresponds to that used for the cells exhibiting the highest efficiency (uniform bandgap).

Fig. 2 shows the effect of $E_{g\max}$ on J_{ph} . The most important point that can be observed is that the photo-generated current density calculated using the effective absorption value (Eq. (2)) in case of a gradual bandgap is higher than for the one obtained for the uniform bandgap case. In addition, the slope of the decrease of photo-current density is smaller in the gradual bandgap case. By comparison with the case of $E_{g\max} = 1.2$ eV, a photocurrent loss (at $E_{g\max}$ around 1.6 eV) of 1.3 mA/cm² and 8.06 mA/cm² is obtained for the gradual and uniform bandgap absorber cases, respectively. This decrease in photocurrent density is linked to the lower probability of photo-generated electrons to be collected due to the electrical field distribution and the increase of the recombination rate at the back contact.

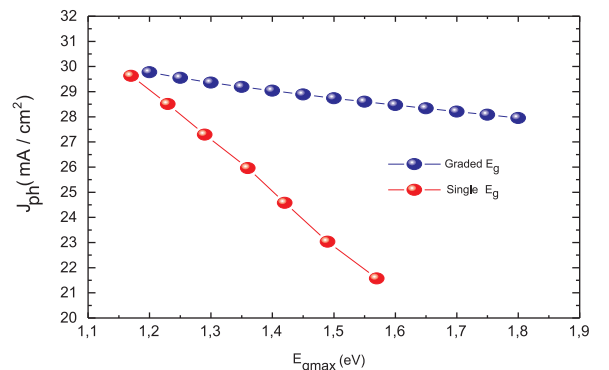


Fig. 2. Variation of photogenerated current density J_{ph} as function of bandgap energy for $d = 2 \mu\text{m}$.

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