Buffer layer optimization for high efficiency CIGS solar cells

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Abstract. This work presents a study concerning the numerical optimization of a buffer layer for high efficiency CIGS solar cells. The dependence of the solar cell properties on the buffer layer material, the layer thickness, the type and density of defects within the same layer were numerically investigated and analysed. Promising results were obtained with alternative Cd-free buffer layers (ZnSnO, InS and ZnS) in place of the standard CdS.

1. Introduction
Among thin-film solar cells based on the I-III-VI semiconductor compound: the polycrystalline Cu(In,Ga)Se₂ (CIGS) absorber layer, is one of the most promising [1,2]. CIGS with its chalcopyrite structure is a direct band gap semiconductor characterized by a high absorption coefficient that allows decreasing the absorber layer thickness in relation to crystalline and multi-crystalline Si solar cells resulting in a reduction of production costs; in fact an active layer with a thickness between 1-2 µm is already enough to guarantee high stability and high efficiencies of the device [3]. Moreover, the use of flexible substrates, in the production flow of these thin film solar cells (e.g. polymer films or stainless steel), have opened new market possibilities. CIGS solar cells grown on polymer film have already demonstrated, at laboratory scale, promising results [4].

In order to enhance the performances of a CIGS solar cell, not only a deep control of the absorber properties is required, but also an optimization of the buffer layer properties is fundamental. Thin film buffer layers grown with different deposition techniques have been extensively studied in the last years. The use of a buffer layer in CIGS solar cell has demonstrated superior performances compared to solar cells without it [5-7]. Several advantages were observed like an evident decrease of the recombination at the interfaces and a reduction of the damages caused by the sputtering of the ZnO layer directly on the absorber [8]. Moreover, since the buffer has usually a refractive index comparable to the one of the ZnO and CIGS layer the reflection losses at the front of the device are kept insignificant.

In order to support the technology development and allow the exploration of new cell/module concepts [9, 10], while meeting specific requirements, we investigated the characteristics of different buffer layers in order to produce highly efficient flexible CIGS solar cells. The chemical bath deposited CdS film is usually employed as buffer layer in a high efficiency CIGS solar cell [11, 12]. The reason of this choice is due to the fact that CdS can cover entirely the rough surface of the CIGS film avoiding the formation of shunt paths [13]. Moreover an efficient heterojunction in ZnO/CdS/CIGS is created; in fact a favorable band alignment can be observed when a CdS buffer layer is used. This work

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investigates the dependence of the solar cells performances on the change of the CdS thickness. Moreover, the influence of the increase of the defects density in the CdS layer was analyzed in order to study its effects on the open circuit voltage (\(V_{OC}\)) and the short circuit current (\(J_{SC}\)) of the final device. Furthermore we investigated, through numerical modelling, the possibility to use alternative buffer layers in place of the standard CdS. The replacement of the CdS by other materials is related to environmental concerns, due to the toxicity of Cd. Additionally, the aim is to increase the short circuit current density of the device by enhancing the photon collection in the region of low wavelength (between 350-550 nm). Since the band gap of CdS is 2.42 eV [14], which corresponds to the wavelength of around 512 nm, only the incident light with a wavelength higher than 512 nm can be transmitted to the absorber layer, resulting in a drop of the quantum efficiency in the high energy region. For this reason the application of a buffer layer with higher energy gap and lower electron affinity, compared to the one of CdS, could result in an enhancement of the solar cell performances reducing the losses in the buffer layer.

2. Simulations

The simulations took account following working conditions: on room temperature, using the solar spectrum AM1.5G as light source incidents on the device. The simulations are based on 1-D electrical model and were carried out using SCAPS, a one-dimensional software package freely available to the PV community [15].

The structure of the simulated CIGS solar cell consists of 200 nm thick n-type ZnO:Al, 80 nm thick i:ZnO, n-type buffer layer (different thicknesses and buffer layer materials were taken account) and a layer of p-type CIGS 1800 nm thick (figure 1).

![Figure 1. Schematic structure of the simulated CIGS solar cell.](image)

The baseline set of the parameters used for the simulations was obtained from in-house measurements performed on each separate layer of the samples and from a study of the data found in literature [16-18]. The numerical model was calibrated with a reference measured CIGS solar cell grown on flexible substrate (reported in [4]). A graded composition of Ga throughout the absorber layer was considered in the simulation. Increased solar cell efficiency was obtained with a double grading profile with a minimum amount of Ga in the middle region of the layer and an increased amount toward the back and the front contacts. In the simulations all the properties, except the ones of the buffer layer, were kept unchanged in order to be able to analyse only the influences of the changes in the buffer layer and their effects on the solar cell parameters. The buffer layer optimization, performed through the simulations, was done in the following steps:

1) variation of the CdS thickness to find out the optimal value taking into consideration the technological constraints, such as the difficulty to grow a uniform thin CdS layer using chemical bath deposition process, properly covering the rough surface of the absorber layer,

2) variation of the defects properties in the CdS layer in order to identify how much the performances are influenced by the change of the defects density and the defects energy level,
3) replacement of the CdS layer with a Cd-free buffer layer in order to investigate the possibility to use alternative buffer enhancing the device performances.

2.1 CdS layer thickness

The CdS layer thickness was varied from 10 nm to 80 nm. The results of the simulated current density vs. voltage (I-V) and external quantum efficiency (EQE) curves for different CdS thicknesses are reported in figure 2.

As shown in the figure 2, the influence of the change of the CdS thickness is more evident from the EQE curves. It can be observed that a rise of the buffer layer thickness causes a drop of the blue response of the EQE due to the increased absorption in the CdS layer. Moreover, it should be considered that a thickness of around 10 nm represents a limit for the buffer layer thickness [19]. Under this thickness the buffer will not compensate the degradation effects of the rough surface of the polycrystalline CIGS layer and these effects will not be any longer negligible. In figure 3 the solar cell parameters at different CdS thicknesses are shown. It is evident from the results that the open circuit voltage ($V_{OC}$) and the fill factor (FF) are just slightly influenced by the change on the CdS layer. On the contrary its influence on the short circuit current ($J_{SC}$) and consequently on the efficiency ($\eta$) is more accentuated. An exponential decrease of the $J_{SC}$ was observed and shown by an exponential fitting line in figure 3. A too thick CdS layer will increase absorption in the buffer layer itself causing a decrease of the incident photons reaching the active layer and an increment of the recombination of the minority carriers that causes the reduction observed in EQE curves between 350 and 500 nm. The simulations reported on this paper showed that the preferred thickness of CdS layer is around 20 nm, the future challenge for the material developers will be to grow such a thin, uniform, adherent, and reproducible large area CdS layer with a good quality using chemical bath deposition or other techniques.
2.2 CdS defects density and defects energy level

The impacts of the traps properties in the CdS layer on the solar cell defects density and defects energy level in the bulk or at the interface with the CIGS layer was evaluated. As the first approach the defects density in the bulk region of the buffer layer 50 nm was varied in order to investigate its effects on the solar cell parameters. The results can be observed in the I-V and EQE curves simulated and presented in figure 4.

Figure 3. Effects of the CdS thickness change on the solar cell performances.

Figure 4. Simulated I-V (left) and EQE (right) curves for different CdS defects density in the bulk region. The total density of traps was varied from $10^{14}$ to $10^{18}$ cm$^{-3}$. 
From figure 4 it is evident that the rise of the defects density brings to a deterioration of the solar cell performances as shown in the simulated I-V curves and in the spectral responses. An increase of the total trap density of the acceptor-like mid-gap defects in the bulk region of the CdS layer will cause an enhancement of the recombination processes. In order to evaluate also the impacts of the interface defects on the solar cells, the same simulations were carried out considering variable defect densities at the interface with the absorber layer instead of the middle gap defects. For the simulation of the interface defects a surface defect layer (SDL) with optical properties similar to the CIGS layer was considered. The SDL band-gap, the electron affinity and the defects concentration were varied. The obtained results are presented in figure 5. The performed simulations show that the changes in the defects density have more influence on the solar cell performances than the position of the traps in the buffer layer. In fact the interface and bulk defects present the same behaviour and effects on the solar cell performances in the majority of the simulated range of the traps densities. Only for the defect densities over $10^{17}$ cm$^{-3}$ the defects located in the bulk of buffer layer have more impact on the deterioration of the solar cell parameters than the defects on the buffer/absorber interface. The rise of the interface or bulk defects density in the buffer layer deteriorates the $J_{SC}$ without significantly affecting the $V_{OC}$.

![Figure 5. Effects of different trap densities at the interface, between buffer and absorber layer, and in the bulk region on the performances of the solar cell.](image)

2.3 New buffer layer

Three different alternative buffer layers (ZnSnO (ZTO), InS and ZnS) were modelled in order to check the possibility to replace the CdS with a non-toxic material characterized by higher energy gap in order to overcome the photocurrent losses that characterize the use of the CdS layer. Different technique of growth can be used to produce and test new buffer layer material and in this work, the transmittance data of the three different sputtered buffer layers were considered. The transmittance curves of the alternative buffer layers, are presented in figure 6 and were used as input data for the calculation of the absorptions at different wavelengths used in the model.
Figure 6. Transmittance measurements of three alternatives Cd-free layers used as input in the simulations.

In the model three new materials used as buffer layer were simulated considered a higher electron affinity and energy gap compared to the CdS. In particular a 3.0 eV energy gap was used and 100 nm thick buffer layers. The resulted I-V and EQE curves obtained from simulations are reported in figure 7.

Figure 7. Simulated I-V (left) and EQE (right) curves for three different sputtered new buffer layers: ZTO, ZnS and InS.

As shown in the simulations results the most promising Cd-free buffer is the ZTO, having the best I-V curve and the highest spectral response. A comparison among the simulated solar cells performances using different buffer layers and the reference cell with CdS is presented in table 1.

Table 1. Solar cell parameters obtained from simulations using three different sputtered buffer layer and a CdS layer for comparison.

| Buffer layer used in the simulation | V\text{oc} (mV) | J\text{sc} (mA/cm}^2 | FF (%) | η (%) |
|------------------------------------|----------------|----------------------|-------|------|
| CdS                                | 702            | 37.3                 | 74.7  | 19.5 |
| ZTO                                | 704            | 38.6                 | 75.0  | 20.3 |
| ZnS                                | 702            | 37.5                 | 75.0  | 19.7 |
| InS                                | 698            | 33.6                 | 74.9  | 17.6 |
As reported in table 1 using ZTO and ZnS as buffer layer enhances the short circuit current and consequently the efficiency. On the contrary the open circuit voltage and the fill factor are just slightly influenced by the change of the buffer layer.

3. Conclusions
In this work we simulated the effect of the different buffer layer properties (thickness, defects, materials) on the performance of the CIGS solar cell in order to find the optimal configuration. The simulations show that the best performances in a CIGS solar cell, using a CdS layer, are obtained for a 20 nm thick buffer. The simulation results suggested that the interface and bulk defects in the CdS layer have similar influence on the solar cell performance. In both cases a deterioration of the short circuit current is observed while just a slightly change in the open circuit voltage is showed. Moreover simulations have also demonstrated the possibility to use alternative buffer layer instead of CdS, obtaining promising results especially with the ZTO layer. Further experimental work will be carried out in order to confirm the presented simulation work.

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