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Optimisation of rear reflectance in ultra-thin CIGS solar cells towards >20% efficiency

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ABSTRACT

In order to decrease their cost and the use of rare metal elements, thin film solar cell thicknesses are continuously reduced at the expense of their efficiency, due to a lack of absorption for long wavelengths. Optimisation of cells rear reflectance (R_b) thus becomes meaningful to provide non-absorbed light a second chance to be harvested by the active cell layer. In this sense, we present a way to keep the rear reflectance in advanced Cu(In, Ga) Se₂ (CIGS) cell as high as possible while keeping in mind the progress already done regarding the rear passivation techniques. We show that introducing a stack of thin Al₂O₃ and aluminium between the CIGS layer and the rear molybdenum electrode increases R_b up to 92% in the long wavelength 800–1100 nm range. Several other stacks, using MgF₂, SiO₂ or TiO₂, are optimised in order to investigate the best trade-off between passivation, material consumption and performances, resulting in R_b ranging from 42% (moderate case) to 99% in the best case. Those CIGS rear interface reflectance optimisations were performed by using a standard transfer matrix method (TMM) in the long wavelength range. Seven interesting stacks are then analysed for solar cell performances using SCAPS simulation software to understand the impact of rear reflectance on short circuit current density (J_{sc}) and eventually on the cell efficiency (η), for ultra-thin CIGS absorber thicknesses (<1 μ m). Based on these results, we propose R_b optimisation to achieve $J_{sc} > 40$ mA/cm² and $\eta > 20\%$ with a 500 nm-thick CIGS absorber film using CIGS-Al₂O₃-Mo stack, where the Al₂O₃ thickness can be chosen in between 104 and 139 nm. This way, we can ensure good rear reflectance ($R_b = 65\%$) and reduced interface recombination while being industrially feasible with present technologies.

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1. Introduction

CIGS solar cells are presently considered to be the best thin film absorbing material in terms of their excellent light-to-power conversion efficiencies exceeding 20% (Ramanathan et al., 2003; Jackson et al., 2011). Unfortunately, their use of rare metals is a challenge when aiming for a long-term marketability. Since other industrial applications (e.g., LED, high-frequency transistors, infrared detectors, ...) also use gallium and indium, which are in short supply, it is of the utmost importance to reduce their use if CIGS thin-film solar cells are to be produced in large volumes. While moving towards ultra-thin (± 500 nm) CIGS solar cells will reduce the costs and thus bring economic advantages, it will also induce a loss of absorption within the cells (Andreani et al., 2012). Optimising the rear reflectance (R_b) to give light a second chance to be absorbed while taking into consideration the highly recombinative CIGS/Molybdenum (Mo) rear contact interface is then mandatory in order to retain high efficiency devices (Krc et al., 2016).

Although rear interface passivation is already addressed by using aluminium oxide (Al₂O₃) (Vermang et al., 2014b,c; Kotipalli et al., 2015b, in press), efforts are still needed to improve R_b . Up to now, the most interesting approach is to use nano-structures (Ji et al., 2013; Bednar et al., 2015; Yin et al., 2016) or nano-particles on the rear side to build a highly reflective structure which scatters the light back into the CIGS layer (Vermang et al., 2015a; Lare et al., 2015). Although these methods are very effective, their optimisation and their homogeneity on large areas are still a challenge. Some studies have already shown that replacing molybdenum with gold or silver improve the rear reflectance, thus increasing the cell performances (Dahan et al., 2012; Li-Kao et al., 2012). Other metals like W, Cr or Ta (Orgassa et al., 2003a), zirconium nitride (ZrN) (Krc et al., 2016; Schleussner et al., 2009) or titanium nitride (TiN) (Mahieu et al., 2011) have been tested and have shown good results. The backwall supersaturate structure, where the glass substrate is used as the front-part of the device, gives an other effective alternative to improve ultra-thin film solar cell performances by using silver (Ag) reflector on the rear side (Larsen et al., 2014; Simchi et al., 2014).

We propose with this work an alternative industrially viable and scientifically interesting method using optimised rear material stacking instead of complex photonics nano-structures. This means, by the use of few layers of dielectric and metal using industrial or other de-

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position techniques, we can achieve similar R_b while simultaneously providing the rear surface passivation and an excellent diffusion barrier against elements moving from the base substrate (especially stainless steel) during the high temperature process step.

In this work, rear reflectance optimisation is addressed by using a transfer-matrix method. These methods are well-known in thin-film optics to investigate optical properties of material stacks (Hass and Gerstenberg, 1964; Pedrotti and Pedrotti, 1993; Angus Macleod, 2001). The method allows the study of R_b , that is the amount of light reflected back into the CIGS, independently of the rest of the cell. The impact of R_b on the current density (J_{sc}) and cell efficiency (η) is then addressed by incorporating the transfer matrix results in a 1-D Solar Cell Capacitance Simulator (SCAPS, University of Ghent, Belgium), to give guidelines for cells fabrication.

This article is divided in two parts. The first part exposes the theoretical optical issues when CIGS thickness is reduced and presents succinctly the transfer matrix method used in this work, necessary to support the results and the discussion. The second part of this work presents the effect of some optimised thin-film stacks from the first part on the global CIGS cell parameters (J_{sc} and efficiency) by using SCAPS.

2. Optical simulations

In the following Sections 2.1–2.5, we go through CIGS rear reflectance optimisation and highlight the best stacks studied here. All the material optical parameters to study a CIGS cell can be found in Orgassa et al. (2003b), Han et al. (2004), Chen et al. (2015), Rubio-Bollinger et al. (2015), Bernal-Correa et al. (2016), and Onwudinanti et al. (2016) and are summarised in the supplementary data.

2.1. CIGS absorption

Optical properties of materials are mainly explained by their complex refractive index $\tilde{n}(\lambda) = n(\lambda) - ik(\lambda)$, where n is the real refractive index and k is the extinction coefficient, both being a function of λ , the wavelength at which materials are exposed. The extinction coefficient governs how the spectral irradiance is decreasing while the light propagates through the material. This is expressed through the Lambert-Beer's law as

$$\frac{I(\lambda)}{I_0(\lambda)} = e^{-\alpha z} \quad \text{with} \quad \alpha = \frac{4\pi k}{\lambda}$$

where $I(\lambda)$ is the irradiance after a propagation length z (in metre) in

the medium, $I_0(\lambda)$ is the initial spectral irradiance and α is the absorption coefficient. In a medium free from absorption, $k(\lambda) = 0$ while it can reach high values in absorbing media such as metals or semiconductors.

Computing this equation for CIGS material using the AM1.5 D solar spectrum as $I_0(\lambda)$ shows that CIGS is an excellent absorber compared with silicon (Fig. 1a), due to its direct bandgap. A 1 μm -thick CIGS is already enough to absorb 97% of the input irradiance for wavelengths comprised between 300 and 800 nm, while silicon exhibits the same behaviour only between 300 nm and 434 nm (Fig. 1b). This statement does not hold true for long wavelength. In the case of 1 μm -thick CIGS, wavelengths above 800 nm become less and less absorbed until the corresponding energy is equal to the bandgap energy. This absorption loss becomes really critical for thicknesses below 1 μm (Fig. 1) because a substantial part of the input irradiance is not fully absorbed, thus decreasing the external quantum efficiency (EQE) of the device. Managing rear reflection (R_b) while decreasing the active thickness in ultra thin CIGS cells thus becomes mandatory to keep the efficiency as high as possible (Vermang et al., 2014b; Kotipalli et al., in press).

2.2. Theoretical background

In thin-film optics, the ratio between the magnetic field amplitude H and the electric field amplitude E of a single linearly-polarised plane wave in a non-magnetic ($\mu_r = 0$) medium is given by

$$\frac{H}{E} = y = \tilde{n}Y_0$$

where y is the characteristic optical admittance of the medium, $\tilde{n}$ the complex refractive index and $Y_0 = \sqrt{\frac{\epsilon_0}{\mu_0}}$ the admittance of the free space (Angus Macleod, 2001). Reflection on a diopter at normal incidence is simply given by

$$r = \frac{y_0 - y_s}{y_0 + y_s} \quad \text{and} \quad R = r \cdot r^*$$

where r is the reflection coefficient, R the reflectance, y_0 the characteristic admittance of the incident medium and y_s the characteristic admittance of the substrate. A high contrast between y_0 and y_s will give a high reflectance.

When the admittances are replaced by their definitions, we come back to the well-known Fresnel coefficient. In a thin-film system

Fig. 1. (a) AM1.5 D spectral irradiance before and after a propagation through different CIGS thicknesses. The curves are computed using the Lambert-Beer law. The labels correspond to the propagation length (z). (b) Relative absorption of the solar spectrum by CIGS. This graph shows the amount of light already absorbed by the CIGS. Silicon (red line) is added as a reference. Front reflection and diffusion through CIGS losses are not taken into account. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

(Fig. 2), the reflection coefficient keeps the same form (Angus Macleod, 2001),

$$r = \frac{y_0 - Y}{y_0 + Y}$$

but Y is now the input optical admittance of the system and is defined by H_1/E_1 where $H_1(E_1)$ is the amplitude of the magnetic field (electric field) at the input interface (denoted by 1 in Fig. 2). The input fields are linked with the output fields through a characteristic matrix M which only depends on the thin-film parameters (Hass and Gerstenberg, 1964; Pedrotti and Pedrotti, 1993):

$$\begin{bmatrix} E_1 \\ H_1 \end{bmatrix} = M \begin{bmatrix} E_2 \\ H_2 \end{bmatrix} = \begin{bmatrix} \cos \delta & \frac{i}{y_1} \sin \delta \\ iy_1 \sin \delta & \cos \delta \end{bmatrix} \begin{bmatrix} E_2 \\ H_2 \end{bmatrix}$$

where y_1 is the thin-film characteristic admittance and $\delta = 2\pi y_1 d / \lambda$ is the phase factor due to the physical thickness d of the film. By normalising the fields by E_2 , we get:

$$\begin{bmatrix} E_1/E_2 \\ H_1/E_2 \end{bmatrix} = \begin{bmatrix} \cos \delta & \frac{i}{y_1} \sin \delta \\ iy_1 \sin \delta & \cos \delta \end{bmatrix} \begin{bmatrix} 1 \\ y_s \end{bmatrix}$$

We can then express the input admittance Y as a function of the thin-film parameters and the substrate admittance:

$$Y = \frac{H_1}{E_1} = \frac{y_s \cos \delta + iy_1 \sin \delta}{\cos \delta + i \frac{y_s}{y_1} \sin \delta}$$

If the thin-film is replaced by a multilayer, the characteristic matrix of the system is the product of the characteristic matrices of all layers $M = M_1 M_2 \dots M_n$. TMM consists to compute M the characteristic matrix of the studied system to obtain r then R .

The foregoing is always valid as long as the incident material is free from losses, *i.e.* y_0 is real (for non-absorbing medium). When y_0 becomes complex, as it is the case when analysing the rear side of a solar cell, the reflectance cannot be theoretically defined by $R = r \cdot r^*$ anymore because the incident irradiance and the reflected irradiance are now coupled together (Angus Macleod, 2001). The coupling term is called the mixed Poynting vector (Macleod, 2014) and is essentially an interference term. Ignoring this term by using R as it is defined above could lead to $R_b > 1$ in some cases, which is obviously

unphysical (see Fig. 3 in supplementary data). On the other hands, the reflection coefficient r is still valid.

It is interesting here to raise this theoretical issue because softwares like SCAPS (Khoshsirat and Yunus, 2013; Mostefaoui et al., 2015) still require to provide a rear reflectance (R_b), which cannot be defined in absorbing media. Fortunately, the mixed Poynting vector will only be important with high extinction coefficient, *i.e.* when the incident irradiance will be absorbed anyway, before reaching the rear side. In fact, the mixed Poynting vector is, in the best interference condition, of about $2 \frac{k}{n} \sqrt{r \cdot r^*}$ (Macleod, 2014). On the other hand, it will not be important when k is small and n is high enough, as it is often the case for semiconductors in long wavelength, especially for CIGS in the 800–1100 nm range. In this work, we thus set the extinction coefficient of CIGS k_{CIGS} to zero so that $R = r \cdot r^*$ is valid but tainted with a small error proportional to the mixed Poynting vector.

That being said, the validity of the results obtained by setting $k_{CIGS} = 0$ can be checked by looking at the transmittance instead of the reflectance. We know from the perfect absorber concept (Macleod, 2013) that optimising R_b means to cancel light transmission (T) into the substrate. It implies that the exit admittance must be purely imaginary, *i.e.* $\text{Re}(Y) = 0$, that is the locus of Y in the admittance diagram has to cross the imaginary axis, or at least be as close as possible. The computation of the exit admittance does not require to cancel the imaginary part of the incident material refractive index. That will be used in this work to validate the results.

Finally, TMM used here does not explicitly incorporate the effect of the roughness of the layers. It is still possible to take roughness into account in TMM by using statistical representation of the roughness but it depends on the correlation length and needs thorough experimental measurements. More insight could be found in the following literature (Mitsas and Siapkias, 1995; Katsidis and Siapkias, 2002; Tikhonravov et al., 2003; Dahan et al., 2013).

2.3. CIGS rear interfaces

An advanced schematic cross-section of a CIGS cell is shown in Fig. 3a (Vermang et al., 2014a,b,c, 2015a,b; Krc et al., 2006). There are two possible kinds of optical rear interfaces, identified by (1) and (2):

- (1) CIGS-Mo
or CIGS-MoSe₂-Mo
- (2) CIGS-Passivation-Mo

The first interface type is CIGS-rear molybdenum electrode contact. More specifically, a MoSe₂ layer is grown during the selenization step to avoid Schottky barrier (Schlenker et al., 2007) and to ensure an ohmic contact between CIGS and Mo (Cao et al., 2011). The second interface is formed by a passivation layer between CIGS and Mo.

The passivation layer will mostly be alumina (Al₂O₃) due to its field-effect passivation (Vermang et al., 2014c; Kotipalli et al., 2015b, in press) and is then mainly studied in this work. It should be noticed here that we only focus on the relative rear reflectance (R_b) of optical interfaces. Absolute reflectance could be obtained by multiplying the residual irradiance at the rear interface (see Fig. 1a) by the relative reflectance.

The wavelength range selected here corresponds to long wavelength between 800 and 1100 nm. We first point out from Fig. 3b that reflection on CIGS-Mo interface is low (around 30%, dashed curve). In general, bare Mo is not an effective reflector, only reflecting about 65% of the light while aluminium reflects more than 90% (Fig. 3b). It becomes even worse when growing the necessary MoSe₂ (Fig.

Fig. 2. Thin film model used in transfer matrix. An example of corresponding materials are indicated between brackets.

Fig. 3. (a) Schematic cross-section of a CIGS cell. Aluminium-doped zinc-oxide (AZO) is ZnO:Al. (b) Relative reflectance of few optical interfaces. Thin-film thicknesses are set to 50 nm for Al_2O_3 and 20 nm for MoSe_2 . (1) and (2) show two different interfaces in (a) and their respective reflectance in (b).

3b). This growth drastically increases matching between exit $Y_s^{\text{MoSe}_2-\text{Mo}}$ and input Y_0^{CIGS} admittance, which acts as an anti reflective coating (ARC, Fig. 4). The worst case is 22.4 nm of MoSe_2 , where its locus crosses the real admittance axis.

On the other hand, adding a dielectric layer, such as amorphous Al_2O_3 between CIGS and Mo, increases the amount of light reflected back into CIGS (Fig. 3b). In the admittance diagram, increasing Al_2O_3 thickness does not change a lot the contrast between exit and input admittances but it drastically decreases the real part of Y_s (Fig. 4), thus decreasing T into Mo and improving R_b . The last statement remains true as long as the layer between CIGS and Mo is transpar-

ent, where $R + T = 1$ ($R + T + A = 1$ otherwise, where A is the absorption within the intermediary layer). The optimum Al_2O_3 thickness that maximises R_b at 900 nm is then 117.6 nm. Only part of the admittance loci are plotted in Fig. 4 to make it easier to follow. Full locus for a dielectric is a circle traced in clockwise direction and centred on the real axis.

Although admittance diagram is a convenient way to optimise dielectric thickness as it yields the exact solution at one wavelength, optimising R_b on a range rather than at one wavelength becomes more complex. The following optimisations are thus performed by computing R_b in the selected range. In order to get the best R_b for long wavelength range, we used arithmetic mean $\bar{R}_b(\lambda)$ over the 800–1100 nm range as the performance criteria.

2.4. R_b optimisation

2.4.1. CIGS- MoSe_2 -Mo interface

Growing MoSe_2 is detrimental for $\bar{R}_b$ below 50 nm (Fig. 5a). The worst case happens with a 25.2 nm-thick MoSe_2 where $\bar{R}_b = 10\%$. Above 50 nm, $\bar{R}_b$ becomes higher than bare CIGS-Mo interface and reaches a maximum at 73.6 nm. The optimisation at one unique wavelength (900 nm) gives roughly the same results. The damping behaviour above 85 nm is due to MoSe_2 small absorption around 800 nm.

At 900 nm, the worst case is 22.4 nm of MoSe_2 , which is exactly the thickness found with the admittance diagram.

Reflectance spectra corresponding to worst and best cases are presented in Fig. 5b. R_b is still limited to 50% in the best condition. The problem here is that the MoSe_2 layer thickness is experimentally complex to manage accurately. Moreover, thick MoSe_2 layer also in-

Fig. 4. Admittance diagram at 900 nm, in free space units ($Y_0 = 1$). Only part of the loci are plotted. Arrows show direction of admittance evolution when growing thin films.

Fig. 5. (a) Reflectance of CIGS- MoSe_2 -Mo interfaces depending on the MoSe_2 thickness, at 900 nm and its average on the 800–1100 nm range. (b) Reflectance spectrum of CIGS- MoSe_2 -Mo interfaces for the best/worst MoSe_2 thickness. Bare CIGS-Mo spectrum is given as a reference.

duces a series resistance R_s , thus reducing the cell fill factor (FF) and efficiency (Polizzotti et al., 2013; Lin et al., 2016).

Decreasing CIGS-MoSe₂-Mo interface area by using point-contact instead of full metal contact on the rear side is considered to be one of the best options (Vermang et al., 2014a,c). This method is already used in silicon PERC-family in order to decrease contact resistance and to reduce rear surface recombination velocity (S_b , rear SRV).

2.4.2. CIGS-passivation-Mo interface

Passivation layers are used in silicon cells in order to decrease the SRV of the minority carriers and to minimise the optical losses on front and rear sides of a cell (Kotipalli et al., 2013a). In the case of a p-type semiconductor, Al₂O₃ is widely used for its chemical and field effect passivations due to its high negative charge density (Agostinelli et al., 2006; Hoex et al., 2008; Terlinden et al., 2010; Werner et al., 2011; Kotipalli et al., 2013b) as well as a barrier against diffusion (Van Delft et al., 2012).

Adding Al₂O₃ between CIGS and Mo greatly increases $\bar{R}_b$ (Fig. 6a). The best case corresponds to an Al₂O₃ thickness of 121 nm while the worst case happens at 268 nm, resulting in a mean rear reflectance $\bar{R}_b$ of 65% and 31% respectively. As it is the case for MoSe₂, optimisation at 900 nm gives a thickness of 117.6 nm, the solution found with admittance diagram (Fig. 4). This highlights that optimising dielectric thickness with either the admittance diagram or by computing $\bar{R}_b$ with the extinction coefficient of the incident medium set to zero brings the same solutions. The only thing that could be altered is the absolute value of R_b .

Reflectance spectrum corresponding to worst and best cases for Al₂O₃ are presented in Fig. 6b. The worst case gives approximately the same $\bar{R}_b$ than the bare interface, that is CIGS-Mo interface. Adding Al₂O₃ is then always profitable, at least for the sake of the passivation.

Thickness variation around the best case is not a problem and allows inaccuracy during the deposition.

In fact, thickness in a 104–139 nm range still reflects more than 64%. This 14%-error on the thickness is by far greater than a standard coating-system accuracy (around 10%).

Although Al₂O₃ is one of the best materials for passivation, a few others are of great interest from a research point of view: magnesium fluoride (MgF₂) and silicon dioxide (SiO₂) for their low characteristic admittance (or low refractive index) and titanium dioxide (TiO₂) for its diffusion barrier capability (Paz and Heller, 1997; Finley and Gillery, 1998; Uerantassun et al., 2003). Evolution of $\bar{R}_b$ with thickness for these 3 dielectrics are shown in Fig. 7a and their respective best spectra in Fig. 7b.

Out of the four dielectrics, MgF₂ gives the best $\bar{R}_b$, about 72% for a thickness of 144 nm. On the other hand, TiO₂ is the worst material, with a maximum $\bar{R}_b$ of 42%. Best case for each material are summarised in Table 1. The thickness analysed here corresponds to thickness around the quarter-wave condition at 900 nm. Even with MgF₂, $\bar{R}_b$ is still relatively low due to the non-appropriated optical admittance of Mo. Finishing the stack with an effective metal reflector such as aluminium is thus mandatory to reach higher $\bar{R}_b$.

In the following, a 15 nm-thick layer of Al₂O₃ is kept on the CIGS rear interface for passivation purpose, as it is often done experimen-

Fig. 6. (a) Reflectance of CIGS-Al₂O₃-Mo interfaces depending on the Al₂O₃ thickness, at 900 nm and its average on the 800–1100 nm range. (b) Reflectance spectrum of CIGS-Al₂O₃-Mo interfaces for the best/worst Al₂O₃ thickness. Bare CIGS-Mo spectrum is given as a reference.

Fig. 7. (a) Average rear reflectance versus dielectric (passivation) thickness, for 4 materials. The vertical lines are guidelines to indicate the optimised thicknesses. (b) Rear reflectance of the optimised dielectric-thickness from (a), for the 4 materials. Bare CIGS-Mo spectrum is given as a reference.

Table 1

Material and thickness optimisation of $\bar{R}_b$, defined as being the average R_b on 800–1100 nm wavelength range. C = CIGS, M = MgF_2 , T = TiO_2 . #Layers is the number of layers between CIGS and Mo. Thickness(es) is/are the thickness(es) of the dielectric layers between CIGS and Mo. $\text{Re}(Y_s)$ is the real part of the exit admittance (at 900 nm). d_{range}^e is the dielectric thickness range for which 99% of $\bar{R}_b$ (last column) can be obtained and ϵ the maximum related error allowed (compared with the maximum one). d_{Al} is the minimum aluminium thickness to get 99% of the max $\bar{R}_b$ (last column), obtained with 90 nm-thick Al in the simulations.

Case N. & stack	#Layers	Thickness(es) [nm]	$\text{Re}(Y_s)$	d_{range}^e [nm]	d_{Al} [nm]	$\bar{R}_b$ [%]
<i>Simple stacks</i>						
1. CIGS-Mo	0	Bare interface	3.063	/	/	33
2. C- TiO_2 -Mo	1	75	0.672	62–88 ^{17.3%}	/	42
3. C- Al_2O_3 -Mo	1	121	0.340	104–139 ^{14%}	/	65
4. C- SiO_2 -Mo	1	135	0.286	115–155 ^{14.8%}	/	69
5. C- MgF_2 -Mo	1	144	0.258	122–165 ^{14.6%}	/	72
6. C- Al_2O_3 - MgF_2 -Mo	2	15–131	0.262	109–152 ^{16%}	/	72
7. C- Al_2O_3 - TiO_2 -Al-Mo	3	15–52	0.139	25–79 ^{52%}	33	86
8. C- Al_2O_3 -Al-Mo	2	126	0.069	88–165 ^{30.2%}	28	92
8'. C- Al_2O_3 -Cu-Mo	2	122	0.021	58–183 ^{24.6%}	45 ^{Cu}	97
8''. C- Al_2O_3 -Ag-Mo	2	124	0.011	43–203 ^{63.7%}	43 ^{Ag}	98
9. C- Al_2O_3 - SiO_2 -Al-Mo	3	15–126	0.058	82–170 ^{34.9%}	26	93.5
10. C- Al_2O_3 - MgF_2 -Al-Mo	3	15–135	0.053	88–182 ^{34.8%}	25	94
<i>Bragg multilayer stacks</i>						
11. C- Al_2O_3 -MTM-Mo	4	15-M149-T99	0.096	/	/	88
12. C- Al_2O_3 -MTMTM-Mo	6	15-M154-T101	0.036	/	/	94
13. C- Al_2O_3 -MTM-Al-Mo	5	15-M150-T98	0.019	/	17	98
14. C- Al_2O_3 -MTMTM-Al-Mo	7	15-M155-T99	0.007	/	10	99

tally. This layer is small enough to avoid bad optical impact and thick enough for the field effect to be effective (Kotipalli et al., 2013a). Adding this layer between CIGS and MgF_2 doesn't change $\bar{R}_b$ (still 72%) but decreases the optimum MgF_2 thickness down to 131 nm (Fig. 8a & b). This is the best trade-off regarding the optical losses, passivation and materials thickness.

On the other hand, a thin aluminium layer between dielectrics and molybdenum greatly enhances rear reflection. The stack CIGS- Al_2O_3 -Al-Mo (stack 8 in Table 1) improves $\bar{R}_b$ up to 92%.

Adding the same aluminium layer on the previous best option (stack 6) improves $\bar{R}_b$ up to 94%, where the stack is CIGS- Al_2O_3 - MgF_2 -Al-Mo (stack 10) in this case (Fig. 8a & b).

Fig. 8. (a) Average rear reflectance versus dielectric (passivation) thickness, for 4 different stacks. (b) Rear reflectance of the optimised dielectric-thickness for the 4 stacks.

Aluminium layer could be ultra thin as 99% of the two previous $\bar{R}_b$ are already obtained with 27 nm and 25 nm-thick Al respectively, while reaching $\bar{R}_b$ of 92% and 94% for 70 nm and 63 nm.

We kept in simulation Al-thickness to 90 nm (thick enough to optically act as bulk metal) in each case to get the highest achievable $\bar{R}_b$. The thickness to reach 99% of this value is then indicated in Table 1.

The optimum thickness of each dielectric layer are slightly modified by adding the 15 nm-thick Al_2O_3 and the ultra-thin Al layer. All these results are summarised in Table 1.

TiO_2 becomes optically interesting when adding an Al layer. Indeed, the stack CIGS- Al_2O_3 - TiO_2 -Al-Mo gives $\bar{R}_b = 86\%$ at the optimum thickness of 52 nm (Fig. 8a & b). The stack CIGS- Al_2O_3 - SiO_2 -Al-Mo gives $\bar{R}_b = 93.5\%$, thus being the second best solution (Not traced on Fig. 8 for visibility purpose). The ultra-thin Al layer could easily be added in the already existing bottom-up process (Vermang et al., 2014a).

The stack 8 has also been simulated with copper (Cu) and silver (Ag) instead of aluminium. The results are summarised in Table 1 as stack 8' and 8''. These two metals are also promising due to their high reflectance in infrared (IR) region. On another hand, gold (Au) has also demonstrated excellent reflective properties in the IR-region, but is expensive for large scale industrial production.

2.4.3. CIGS-multilayer-Mo interface

Although periodic stacks (Bragg mirror) are known to improve reflectance, it is not worth to add many layers to gain few % more. We limited our analysis at 5 layers maximum. The stacks have the following structure: CIGS- Al_2O_3 -L-(Al)-Mo, CIGS- Al_2O_3 -LHL-(Al)-Mo and CIGS- Al_2O_3 -LHLHL-(Al)-Mo, with or without Al, where L stands for Low (admittance or refractive index) and H stands for High. A higher contrast between L and H will result in higher performances, so that the only interesting case here is L = MgF_2 =M and H = TiO_2 = T.

Thickness optimisation leads to $\text{MgF}_2 = 149$ nm/ $\text{TiO}_2 = 99$ nm (Fig. 9a) with $\bar{R}_b = 88\%$ for LHL stack and $\text{MgF}_2 = 150$ nm/ $\text{TiO}_2 = 97$ nm (Fig. 9b) with $\bar{R}_b = 98\%$ for LHL-Al stack. We clearly see that an error on the thickness is not detrimental for $\bar{R}_b$. Optimisation for the LHLHL-(Al) stacks gives roughly the same thickness (see Table 1) and is not shown here. All the optimised R_b spectra are presented in Fig. 10.

Increasing the number of layers improves $\bar{R}_b$ but is much less effective than using an ultra-thin Al layer. In fact, the stack CIGS- Al_2O_3 -M-Al-Mo is as good as the very thick CIGS- Al_2O_3 -MTMTM-Mo (Fig. 10). Obviously, the CIGS- Al_2O_3 -MTMTM-Al-Mo stack gives the best performance, with $\bar{R}_b = 99\%$ but is also industrially unrealistic (costly and low throughput).

Fig. 9. $\bar{R}_b$ optimisation versus TiO_2 and MgF_2 thickness for (a) MTM stack and (b) MTM-Al stack. $\bar{R}_b$ iso-contour is set at 2 nm-step in (a) and 1 nm-step in (b).

Fig. 10. Optimised spectra for 6 different stacks, where M = MgF_2 and T = TiO_2 .

2.5. Discussion

Table 1 summarises all the relevant informations from the foregoing simulations. It provides the best $\bar{R}_b$ achievable for all the stacks studied in this work, their respective optimised thickness and the number of layers they are made of. It is clear that decreasing transmission into the substrate by decreasing $\text{Re}(Y_s)$ greatly increase R_b as there is no absorption in the stacks used. The thickness range mentioned in Table 1 is a target-range that ensures to get at least 99% of the optimised $\bar{R}_b$. The most critical case is the stack 3, where the thickness error on Al_2O_3 is limited to 14% maximum. This is still higher than common coating-system accuracy ($\pm 10\%$), which ensures a robust process step. On the other hand, adding a metal thin-layer (Al, Cu or Ag) increases the target-range, allowing the dielectric coating to vary while still keeping a high $\bar{R}_b$.

The bare CIGS-Mo interface (case 1) is bad in the optical point of view. Adding a dielectric between them can already double $\bar{R}_b$ and, the lower its refractive index is, the better it will be (cases 2–5). However, using MgF_2 alone gives only 7% more reflectance at the price of the passivation loss (case 5).

This passivation loss will be even higher if SiO_2 is used alone (case 4), due to its slightly positive charge density. It is thus always recommended to keep at least 15 nm of Al_2O_3 and then use a second low-refractive index material such as SiO_2 or MgF_2 (cases 6–14). Thickness around 15 nm will still be acceptable as it is far away from any quarter-wave conditions. It will slightly modify the optimised thickness presented in Table 1.

Unfortunately, optical constraint due to molybdenum admittance doesn't allow $\bar{R}_b$ to be higher than 72% so that two other alternatives

can be exposed (apart from complex texturization and photonic crystals).

The first solution is to add an ultra-thin IR metal-reflector layer between dielectric and Mo (cases 7–10). The best trade-off here is the stack Al_2O_3 -Al so that only 2 materials are used, while keeping passivation for a relatively good $\bar{R}_b$. Obviously, adding a metal layer in a material stack could lead to thermal problem like delamination. Other kinds of metals can be used for the same purpose as long as their bare reflectivity in long wavelength is high (Ag, Cu, Au, ...). In this work, we focused on aluminium because it is widely used in solar industry and available in a lot of different coating systems. Moreover,

The second solution is to use a Bragg mirror, i.e. a periodical stack of high and low refractive index materials. Although this system is well-known to provide high reflectance, a large number of layers is often needed. In the case of MgF_2 - TiO_2 stack, we need at least 5 layers to become comparable to a dielectric-aluminium stack. Another disadvantage with Bragg mirror is the precise thickness it requires to be fully useful. Even if Bragg mirror could be deposited by atomic layer deposition (ALD) (Poncelet et al., 2015, 2016), it is time consuming and expensive. Fortunately, $\bar{R}_b$ is in this work optimised on a wavelength range rather than on a unique value.

The optimum-thickness map (Fig. 9) shows that error on both thicknesses are acceptable as contours of constant $\bar{R}_b$ are quite large, but it is difficult to set a safety-range because of the ellipse-shape of those contours.

Although it is a common material used in photovoltaic, Si_3N_4 is not considered here because of its high positive charge density ($+Q_p$) which contributes to increase the surface recombination velocity (S_b) (Kotipalli et al., in press). Nevertheless, its moderate refractive index is still interesting from the optical point of view.

It should be noticed that the results presented here may also vary a little bit with the material properties, resulting from different coating techniques used. Nevertheless, the impact will be limited, as it is the case with thickness variation.

3. Solar cell simulations

In this section, we discuss the impact of rear reflectance on the solar cell parameters (J_{sc} and η). This has been achieved by using SCAPS simulation software, where the model accommodates rear dielectric surface passivation effects (i.e. the field effect passivation due to negative fixed charges and interface state densities) using experimentally extracted CIGS/ Al_2O_3 interface properties as described in Kotipalli et al. (in press).

3.1. Opto-electronic simulations

J_{sc} and η are generated for complete CIGS solar cell structure for seven different rear reflectance stacks from Table 1 and four different absorber thicknesses (*i.e.* 250, 500, 750 and 1000 nm). In our simulation model, the rear reflectance files are modified with R_b vs wavelength profiles of the seven proposed stacks. All the simulations were performed under AM1.5 solar spectrum using baseline properties of respective materials provided in Ref. (Kotipalli et al., in press). However, a high quality CIGS film is chosen in our simulation model with improved deep defect concentration of 10^{14} cm^{-3} compared to the present CIGS baseline properties given in Kotipalli et al. (in press) in order to clearly distinguish the optical effect trends. The front surface reflectance is maintained at 5% for all the CIGS thicknesses. The gallium to gallium plus indium ratio $\text{GGI} = \text{Ga}/(\text{Ga} + \text{In})$ of the CIGS absorber (Kotipalli et al., 2015a) is kept at 0.3. The CIGS absorber layers have uniform gallium profiles, in order to avoid complementary optical gains (*i.e.* enhanced band gap). More detailed device mechanisms related to the effects of negative fixed charges, interface trap densities, rear reflectance and their combinations can be found in Kotipalli et al. (in press).

Next, for the sake of clarity only gains related to J_{sc} and η are shown and discussed in order to quantify the impact of R_b only, and not the impact due to the rear surface recombination (*i.e.* improvement in the open-circuit voltage V_{oc} and FF). In the following, we will refer to the reference case, *i.e.* CIGS-Mo, by unpassivated stack (UP-stack, case 1) and the six others by passivated stack (P-stack, cases 3, 6, 7, 8, 10, and 14 in Table 1).

3.2. Discussion

In Fig. 11, UP-stack is considered to be the reference case with no R_b optimisation (*i.e.* $\bar{R}_b = 33\%$), compared to other optimised P-stack with $\bar{R}_b$ ranging between 65% and 98%. More generally, all the stacks show an increasing trend in J_{sc} and cell efficiency with increasing absorber layer thickness. Such gain in J_{sc} is mainly due to the improved optical absorption with increasing absorber thickness. The overall trends in both J_{sc} and efficiencies for thicker absorbers (750 nm and 1000 nm) with rear reflectance beyond 65% can be considered to reach a saturation plateau.

However, for thinner absorber films (250–500 nm), significant gains in the J_{sc} (2.9–4.1 mA/cm^2) are observed with increasing $\bar{R}_b$ (*i.e.* from 65% to 98%). Lesser gains in J_{sc} (0.6–1.2 mA/cm^2) and (0.2–0.6 mA/cm^2) were observed for further increase in the CIGS thickness, *i.e.* from 500 nm to 750 nm, and 750 nm to 1000 nm re-

spectively. It means that a CIGS thickness of 500 nm appears sufficient while considering the rear reflectance optimisation concepts.

For a constant CIGS absorber thickness, the gain in J_{sc} between UP-stack and P-stack 3 is due to both reduced rear surface recombination (S_b) and improved rear reflectance (R_b), whereas the gain obtained between P-stacks 3–14 is solely due to improved R_b . On this note, for a 250 nm CIGS absorber film with improving rear reflectance (from UP-stack to P-stack 3), a considerable gain in both J_{sc} and cell efficiency of 2.2 mA/cm^2 and 6.6% (absolute) respectively were obtained. Such gain in cell efficiency also includes the contribution of improved V_{oc} due to reduced interface and bulk recombinations. This even makes a very thin CIGS film (250 nm) with improved rear reflectance and passivation more effective than a conventional thick one (1 μm) without dielectric (Fig. 11b).

Next, a further improvement in rear reflectance (from P-stacks 3–14) yields gains in J_{sc} and efficiency of 1.6 mA/cm^2 and 0.86% respectively. Similar gain trends were observed for 500 nm absorber films between UP-stack 1 and P-stack 3 with J_{sc} and cell efficiencies of 2.0 mA/cm^2 and 5.79% respectively. Further increase in $\bar{R}_b$ from P-stack 3–14 yields gains in J_{sc} and efficiency of 0.6 mA/cm^2 and 0.33% respectively. Thus overall, we observe a decreasing trend in the gains while moving towards thicker CIGS absorber films even with increasing $\bar{R}_b$ (from UP-stack 1 to P-stack 3 and from P-stack 3 to P-stack 14).

Based on these simulation results and analysis, we confirm that a CIGS thickness of 250 nm is not sufficient to achieve >20% efficiencies even when implementing excellent R_b (stack 7, 98%). The minimum thickness of CIGS target thickness is found to be around 500 nm with moderate to excellent rear reflectance optimisation (P-stacks 3–14: 65–98%).

As a trade-off between the number of stacking materials (*i.e.* process feasibility), gains in J_{sc} and efficiency, we suggest targeting rear reflectance between 65% and 92% to be sufficient for achieving efficiencies >20%. On the other hand, keeping rear surface passivation and industrial feasibility in considerations, targeting Al_2O_3 thickness in a range between 104 nm and 139 nm would ensure $R_b = 65 \pm 0.65\%$ and $\eta > 20\%$.

4. Conclusion

In this work, we investigated the optical properties of a rear CIGS cell interface using rigorously transfer matrix method (TMM) in order to optimise R_b , the rear reflectance. We highlighted the weak reflectance of the standard CIGS-Mo interface and we proposed to use standard thin film stacks to optimise the reflectance, where our performance criteria was $\bar{R}_b$, the average R_b , in the range 800–1100 nm.

Fig. 11. Simulated cell parameters for four different CIGS absorber thicknesses for seven different rear reflectance stacks. (a) Short circuit current density. (b) Cells efficiency. Number 1, 3, 6, 7, 8, 10 and 14 represent the respective stack number in Table 1.

In order to keep the rear CIGS surface recombination velocity (SRV) as low as possible, a fixed 15 nm-thick Al_2O_3 was placed between the CIGS and the dielectric-Mo stack (MgF_2 , SiO_2 , Al_2O_3 or TiO_2). The best achievable $\bar{R}_b$ was 72% by using the stack CIGS- Al_2O_3 (15 nm)- MgF_2 (131 nm)-Mo.

We then proposed to use either an ultra-thin aluminium layer or a multilayer film, bringing $\bar{R}_b$ from 86% with CIGS- Al_2O_3 (15 nm)- TiO_2 (52 nm)-Al (33 nm)-Mo up to 99% with a 5-layers $\text{TiO}_2/\text{MgF}_2$ Bragg stack. The best trade-off between high $\bar{R}_b$, passivation and the number of layers was the stack CIGS- Al_2O_3 (126 nm)-Al (28 nm)-Mo, giving a $\bar{R}_b$ of 92%. We have also shown that other good IR metal-reflector such as copper (Cu) or silver (Ag) provide high rear reflectance.

The impact of $\bar{R}_b$ on cell performance parameters (J_{sc} and efficiency) in function of the CIGS thickness were then performed with SCAPS. We have shown that $\bar{R}_b$ plays an important role in very thin CIGS-thicknesses (thinner than 750 nm) and becomes less detrimental for thicker CIGS. We have also shown that a $\bar{R}_b$ of 65%, standing for a single Al_2O_3 layer of around 121 nm, is already enough to achieve high cell performances, i.e. $\eta > 20\%$ and $J_{sc} > 40 \text{ mA/cm}^2$. Finally, we desired through this work to provide to any researcher the right dielectric thickness ranges to use on a rear CIGS interface in order to get the best performances. Our next step will be to experimentally implement those stacks within our own CIGS fabrication process steps.

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Appendix A. Supplementary material

Supplementary data associated with this article can be found, in the online version, at <http://dx.doi.org/10.1016/j.solener.2017.03.001>.

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