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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) Se_2 (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 Al_2O_3 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 MgF_2, SiO_2 or TiO_2, 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 µm). Based on these results, we propose R_b optimisation to achieve $J_{sc} > 40$ mA/cm^2 and $\eta > 20\%$ with a 500 nm-thick CIGS absorber film using CIGS-Al_2O_3-Mo stack, where the Al_2O_3 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.

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 (Al_2O_3) (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 nanoparticles 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),

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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 deposition 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. 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 $M = M_1 M_2 \ldots M_n$. TMM consists to compute M the characteristic matrix of the studied system to obtain r then R.