A study on the optics of copper indium gallium (di)selenide (CIGS) solar cells with ultra-thin absorber layers

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Abstract: We present a systematic study of the effect of variation of the zinc oxide (ZnO) and copper indium gallium (di)selenide (CIGS) layer thickness on the absorption characteristics of CIGS solar cells using a simulation program based on finite element method (FEM). We show that the absorption in the CIGS layer does not decrease monotonically with its layer thickness due to interference effects. Ergo, high precision is required in the CIGS production process, especially when using ultra-thin absorber layers, to accurately realize the required thickness of the ZnO, cadmium sulfide (CdS) and CIGS layer. We show that patterning the ZnO window layer can strongly suppress these interference effects allowing a higher tolerance in the production process.

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OCIS codes: (050.1950) Diffraction gratings; (160.6000) Semiconductor materials; (230.4170) Multilayers; (310.4165) Multilayer design; (310.6845) Thin film devices and applications; (310.6860) Thin films, optical properties; (350.6050) Solar energy.

References and links
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1. Introduction

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in absorption of sunlight in thinner CIGS layers results in a decrease in current density, as demonstrated experimentally [3,4]. To date, however, no research group systematically studied the effect of variation of the ZnO and CIGS layer thickness on the absorption characteristics of CIGS solar cells. Here we present such systematic study using an in-house program based on finite element method (FEM) to simulate the light interaction with the multilayer cell stack. The absorption characteristics of the CIGS absorber layer are studied as a function of its layer thickness ranging from 2 μm to 100 nm for a large spectral range from 400 nm to 1100 nm. As a thin film multilayer stack, the thicknesses of all individual layers affect the absorption characteristics of the cell. Therefore, the absorption characteristics of the CIGS solar cell with a absorber layer of 500 nm is investigated as a function of the ZnO layer thickness ranging from 200 nm to 500 nm. Using the outcome of the study, we discuss the implications of the reduction of the absorber layer thickness on the production process of CIGS cells. We propose a light management scheme to overcome potential difficulties.

2. Methodology

2.1. FEM for rigorous electromagnetism modeling

An in-house numerical code based on FEM is used to simulate the light interaction with the multilayer stack [5–7]. In brief, FEM solves a boundary value problem for the vector Helmholtz equation for either the electric or magnetic field in a confined computational domain. The computational domain is meshed using triangles or quadrilaterals and the electric or magnetic field is approximated by edge elements of first, second or third order. This method is very accurate and flexible with respect to both material property and shape of geometry.

When used for our study here, since the size of a typical cell module is much larger than the sunlight wavelength, in simulations the cell module can be assumed to be infinitely large. Then a unit computational cell with limited size is defined with a periodic boundary condition in the lateral direction. In the vertical direction, both the top and bottom media are half infinite spaces which are simulated with the so-called perfectly matched layer (PML) [8]. The deposition of ever thinner absorber layers leads to drastic flattening of the interfaces between the layers of the thin/ultra-thin solar cells. For this reason, in this paper the cell stack is modelled as a flat multilayer structure and the basic constitution is shown in Fig. 2. We assume that the essential part of a CIGS cell consists of the following layers: top glass cover, TCO, CdS, CIGS, Mo back contact layer, and glass substrate. In our study, zinc oxide (ZnO) is applied as the TCO layer. The baseline setting of the layer thickness is indicated in Fig. 2. The optical properties...
of ZnO [9] and CdS [10] are cited from references. We refer to [11] for the refractive index of the compound CuIn(0.69)Ga(0.31)Se2 and for being self-contained the data are plotted in Fig. 3. The number of points of mesh is set through a convergence test. In our case 15 points per wavelength provide a consistent accuracy required. The near field information is accurately obtained after running the simulations. Once the field distribution is known, we consider the light absorption in matter as described in the next subsection.

2.2. Absorption in matter

For time-harmonic macroscopic fields:

\[
\mathcal{E} = \text{Re}\left[\mathbf{E}(\mathbf{r})e^{-i\omega t}\right],
\]

\[
\mathcal{H} = \text{Re}\left[\mathbf{H}(\mathbf{r})e^{-i\omega t}\right],
\]

the Maxwell’s equations in matter are:

\[
\nabla \times \mathbf{E} = i\omega \mathbf{B},
\]
\[ \nabla \times \mathbf{H} = -i\omega \mathbf{D} + \mathbf{J}_p, \quad (4) \]
\[ \nabla \cdot \mathbf{D} = \rho_p, \quad (5) \]
\[ \nabla \cdot \mathbf{B} = 0. \quad (6) \]

In the above equations, \( \mathbf{D} = \varepsilon_0 \varepsilon \mathbf{E} \) is the electric displacement, with an electric field \( \mathbf{E} \); and the magnetic induction \( \mathbf{B} = \mu_0 \mathbf{H} \) with a magnetic field \( \mathbf{H} \); \( \mathbf{J}_p \) and \( \rho_p \) are the current and charge densities of the primary source in the media; and \( \varepsilon_0 \) and \( \mu_0 \) are the dielectric permittivity and magnetic permeability of vacuum and \( \varepsilon \) is the relative electric permittivity tensor of the media. For isotropic materials, \( \varepsilon \) reduces to a complex number and can be simply represented by \( \varepsilon \).

The dielectric permittivity can be expressed by the complex refractive index \( \tilde{n} = n + ik \) by,

\[ \varepsilon = \varepsilon' + i \varepsilon'' = \tilde{n}^2 = (n^2 - k^2) + i2nk \quad (7) \]

Expand Eqs. (3) and (4), and we can get:

\[ \nabla \times \mathbf{E} = i\omega \mu_0 \mathbf{H}, \quad (8) \]
\[ \nabla \times \mathbf{H} = -i\omega \varepsilon_0 \varepsilon \mathbf{E} + \mathbf{J}_p. \quad (9) \]

Using the above two equations, one can derive the energy balance in matter:

\[ \frac{1}{2} \mathbf{E} \cdot \mathbf{J}_p = i\omega \left( \frac{\varepsilon_0}{2} \varepsilon \mathbf{E} \cdot \mathbf{E}^* - \frac{\mu_0}{2} |\mathbf{H}|^2 \right) - \frac{1}{2} \nabla \cdot (\mathbf{E} \times \mathbf{H}^*). \quad (10) \]

By integrating the real part of this balance over a volume \( V \) that is enclosed by the surface \( S \) with external normal \( \mathbf{n} \) we obtain:

\[ \int_V \frac{1}{2} \text{Re} (\mathbf{E} \cdot \mathbf{J}_p^*) d^3 r + \frac{i\omega \varepsilon_0}{2} \int_V \varepsilon'' \mathbf{E} \cdot \mathbf{E}^* d^3 r = -\int_S \frac{1}{2} \text{Re} (\mathbf{E} \times \mathbf{H}^*) \cdot \mathbf{n} d^2 r, \quad (11) \]

where \( \varepsilon'' \) is the imaginary part of the tensor \( \varepsilon \). The first term at the left of Eq. (11) is equal to the average rate of increase of mechanical energy in the matter inside \( V \). When there is no primary source (i.e. \( \mathbf{J}_p = 0 \)), this term equals zero. The second term at the left is the average electromagnetic energy that is absorbed inside \( V \). The right-hand side of Eq. (11) is the rate of flow of energy through the boundary of \( V \) into \( V \).

Fig. 4. Configuration of a flat multilayer stack.
In a flat multilayer stack (configuration seen as in Fig. 4), the normal \( \mathbf{n} \) at each interface is \( \hat{z} \) (a unit vector along the \( z \)-axis). With no primary source inside \( V \), Eq. (11) can be simplified to

\[
\frac{\omega \varepsilon_0}{2} \int_{V,n} \varepsilon'' \mathbf{E} \cdot \mathbf{E}^* d^3 \mathbf{r} = - \left( \int_S S_{z,n+1} d^2 \mathbf{r} - \int_S S_{z,n} d^2 \mathbf{r} \right),
\]

(12)

where \( S_z = \frac{1}{2} \text{Re}(\mathbf{E} \times \mathbf{H}^*) \cdot \hat{z} \) is the \( z \)-component of the mean Poynting vector. Now the absorption in a layer \( n \) is equivalent to either side of the equation.

3. Flat multilayer stack

3.1. Basic absorption and reflection spectra

To study the absorption in each layer of the CIGS cell, we simulated the multilayer cell stack for the spectral range from 400 nm to 1100 nm. For the CIGS cell stack as shown in Fig. 2, the reflection and absorption spectra were calculated for normal incidence field from the top. The results are shown in Fig. 5(a). In most studies reported to date, air is chosen as the top incidence medium. For comparison we perform the same calculation to such setting and the results are shown in Fig. 5(b).

Comparing the two frames, we observe that the local maxima of the curves occur at the same positions despite different top incidence medium. The main difference of the two frames is the magnitude of the oscillation of the curves. With air top, the oscillation is stronger which is due to the larger difference in the refractive indices between air and ZnO. Nevertheless it is the same physical phenomenon. Hence, for the systematic study of the effect of variation of the ZnO and CIGS layer thickness on the absorption characteristics of CIGS solar cells, we only discuss the case with glass top cover to avoid redundancy.

At short wavelengths (400 - 500 nm), more than 40% of the incident light is absorbed in the CdS layer. ZnO has an absorption peak around 400 nm and absorbs more than 20% of the incident light. Thus at short wavelength, though the total absorption of the entire cell stack is high, most of the light is absorbed in the ZnO and the thin CdS layer and does not reach the CIGS layer. CdS and ZnO are transparent for wavelength larger than 600 nm, and thus there is no light loss in these two layers. Light absorption in the active CIGS layer peaks around 620 nm.
nm and 850 nm, which is mainly due to the interference effect caused by the 500 nm thick top ZnO layer. In section 3.3, we will show that the position of both peaks depends on the ZnO layer thickness.

3.2. Variation of the CIGS layer thickness

Currently, the standard thin film CIGS solar cell has a CIGS absorber layer of a thickness between 1.5 and 2 \(\mu\)m. Starting with this value, while the CIGS layer thickness is gradually reduced to 100 nm, light propagation in the cell stack is simulated. Then the absorption in the cell and in each consisting layer of the cell is calculated as described in section 2.2. In Fig. 6 the absorption in each layer is mapped out as a function of both wavelength (x-axis) and CIGS layer thickness (y-axis). Moreover, for the CIGS layer thickness thinner than 500 nm, more detailed results are shown in Fig. 7.

As seen from the colormaps in Fig. 6, the light absorption in ZnO and CdS does not depend on the CIGS layer thickness and the absorption is strong for short wavelengths below 600 nm. At the maximum more than 40% light is absorbed in the CdS layer, therefore the light absorption in the CIGS layer is relatively low for that region. As we have discussed in section 2.2, the imaginary part of the dielectric permittivity indicates the absorption capacity of a material. Derived from the dielectric permittivity of CIGS, seen from Fig. 3(b), light absorption efficiency in bulk CIGS decreases monotonically for increasing wavelength. In other words, CIGS becomes more translucent for longer wavelengths. This implies that, to obtain a relatively high absorption, the active layer needs to be optically thick enough to be “opaque” for the entire spectrum of interest. When reducing the CIGS layer thickness from 2 \(\mu\)m to 500 nm, severe optical losses occur in the wavelength range between 700 and 1100 nm. Light in this wave-
Fig. 7. Absorption in ZnO, CdS, CIGS and Mo layers of CIGS cell as a function of wavelength and CIGS layer thickness (from 100 nm to 500 nm). The thicknesses of the layers are: ZnO layer 500 nm; CdS layer 50 nm; and Mo layer 500 nm. The absorption rate is calculated with respect to the total incident field.

Fig. 8. Absorption spectra of the CIGS and Mo layers for varying CIGS thickness.

length range is only partially absorber by CIGS. A large part of the light which is not absorbed in the CIGS layer penetrates the Mo layer and is absorbed in this back contact layer.

However, the light absorbed in the thin CIGS layer in a multilayered stack does not decrease monotonically as the layer thickness reduces. Instead, a quasi-periodic pattern can be observed in the figure, clearly notable in the long wavelength range. This pattern shifts from near-infrared (near 1100 nm) to mid-visible (around 700 nm) progressively as the thickness of the CIGS layer
reduces. This is because light with shorter wavelength experiences a longer optical path length when it passes through the same thickness of a medium, which leads to a higher absorption and fast attenuation of the field. As shown in Fig. 7, the absorption in a CIGS layer of 450 nm thickness is higher than that of a 500 nm thickness. Ergo, high precision is required in the CIGS production process, especially when using ultra-thin absorber layers, to accurately realize the required thickness of all layers in the cell stack.

For a direct comparison between a few interesting values of CIGS layer thickness, the absorption efficiency in the CIGS and Mo layers together with the total absorption in the entire cell stack are shown in Fig. 8.

3.3. Effect of variation of top window layer thickness

Though ZnO [9] and CdS [10] do not absorb light above 600 nm in wavelength, their layer thickness influences the amount of light absorbed in the active layer. The thickness of the ZnO layer determines the primary reflection by the cell stack. When its layer thickness matches the condition such that the reflection from the top and bottom surfaces form a constructive interference, a high reflection occurs. Then a lower amount of light enters the cell stack yielding a lower absorption in the absorber layer. When ZnO layer thickness is such that a destructive interference is formed, a very low reflection occurs, which means that more light enters the cell stack leading to a higher absorption. When the ZnO layer thickness changes gradually, we can observe a periodic change in the total reflection of the cell stack. For a fixed CIGS absorber layer thickness of 500 nm, Fig. 9 displays the total reflection by the cell stack as a function of both the wavelength and the ZnO layer thickness.

![Fig. 9. Total reflection of CIGS cell as a function of wavelength and ZnO layer thickness. Top incidence medium: glass. The thicknesses of the layers are: CIGS layer 500 nm; CdS layer 50 nm; and Mo layer 500 nm. The reflection rate is calculated with respect to the total incident field.](image)

Correspondingly, the absorption in the cell layers is shown in Fig. 10. With changing ZnO layer thickness, the quasi-periodic patterns in the absorption efficiency are clearly displayed. Variation of the thickness of the CdS layer would yield a similar optical effect. Since decrease of the thickness of CdS would lead to a deterioration of the electronic properties of the cell and an increase in thickness would lead to an increase in parasitic absorption, it is not useful to deviate from the current standard layer thickness of 50 nm. Therefore, we decided to not include a variation of the layer thickness of CdS in our study.
4. Light management for thin/ultra-thin film solar cell

Besides the general decline in light absorption efficiency with the reduction of the absorber layer thickness of solar cells, the optics of CIGS cells with (ultra-)thin absorber layers is rather complex due to the fact that the coherence of light becomes effectively important when the layers are optically thin (i.e., comparable to the wavelength). As discussed in the preceding sections, the light absorption efficiency of a thin/ultra-thin solar cell does not decrease monotonically with a reduction in layer thickness. This complexity raises potential manufacturing difficulties, since an accurate control of layer thickness is needed to obtain an optimal cell efficiency and to keep it consistent for cell to cell production. To tackle those issues, an effective light management scheme can assist to redistribute the field inside the cell stack [12–16]. Here we present our contribution on the subject with a preliminary study of the textured TCO top surface.

4.1. Patterning of the TCO

During manufacture of solar cells, roughness can be introduced at the interface of different materials. As has been reported, often those patterns are beneficial for increasing the cell efficiency [17–19]. Most commonly and easily, textures can be fabricated on the surface of the TCO layer [20–22]. For this study, we consider simple grating structures on top of the TCO layer.

On the ZnO top surface, simple structures of trapezoidal/triangular gratings with periodicity along the lateral x-axis are introduced (see Fig. 11). Below the grating, the thickness of the

Fig. 10. Absorption efficiency map in different layers of CIGS cell as a function of wavelength and ZnO layer thickness. Top incidence medium: glass. The thicknesses of the layers are: CIGS layer 500 nm; CdS layer 50 nm; and Mo layer 500 nm. The absorption rate is calculated with respect to the total incident field.
Fig. 11. Constitution of a CIGS cell stack with patterning on the surface of ZnO layer.

Fig. 12. Effect of the structural patterning of the ZnO layer on the absorption characteristics. The top incidence medium is glass. The grating heights (h) are: (a) 50 nm; (b) 100 nm; and (c) 200 nm.

homogeneous ZnO medium is kept at 500 nm. The baseline setting of the CIGS layer of 500 nm is used for this study. We consider a plane wave incident normal to the surface of the cell stack.
To eliminate the polarization effect of a 1D grating, in the simulation we use the combination of the two orthogonal linear polarization states, s- and p-polarizations, i.e. the polarization state is $45^\circ$ to the normal of the grating vector. Gratings with different feature sizes are investigated. The grating parameters are listed in the table next to the geometry of the cell stack in Fig. 11. The absorption characteristics of the cell stack with the three different patterns on the TCO layer are displayed in Fig. 12.

It is clearly shown that with larger feature sizes, the fringes in all the curves get smoother without decrease of absorption. This is because patterning the ZnO layers causes diffraction of the field, breaking the standing wave patterns formed because of the flat multilayer system. To illustrate this, we compared the near field distribution, in Fig. 13, of the reference cell without grating and the cell with grating ($h = 200$) for light of a wavelength of 750 nm. With the grating, we can see in Fig. 13 the field around the structure is disturbed by the geometry. A z-component of the electric field ($E_z$) is generated because of the structure, whereas in the flat multilayer stack, it is absent. That means part of the light is propagating along the lateral direction of the cell stack. Though this effect is confined to the short vicinity of the structure, it still enhances the field inside the cell stack reducing the reflection. The result is an increase in the absorption inside the absorber layer for this specific wavelength. The diffraction effect is stronger with larger feature size as one would expect, which leads to smoother curves.

We conclude here that patterning the ZnO layer is preferable for having a uniformly high absorption efficiency of the active layer. However the patterning discussed here does not enhance the overall absorption efficiency. To increase the light absorption for wavelengths above 700 nm, it is necessary to continue to focus on other strategies for achieving this goal.
nm, further investigation on light management structures is needed.

5. Conclusions

We presented a systematic study on the effect of variation of the ZnO and CIGS layer thickness on the absorption characteristics of CIGS solar cells using a simulation program based on FEM. We showed that in the wavelength regime between 400 and 500 nm, most of the incident light is absorbed in the ZnO and CdS layers. For wavelengths above 600 nm, both layers are transparent allowing more light to penetrate into the CIGS layer. When reducing the CIGS layer thickness from 2 \( \mu \text{m} \) to 500 nm or less, we observed significant optical losses, mainly in the wavelength region between 700 and 1100 nm. A significant part of the light in that wavelength regime is absorbed in the Mo layer. Our study has shown that the absorption in the CIGS layer does not decrease monotonically with its layer thickness due to interference effects. Ergo, high precision is required in the CIGS production process, especially when using ultra-thin absorber layers, to accurately realize the required thickness of the ZnO, CdS and CIGS layer. We showed that patterning the ZnO window layer can strongly suppress these interference effects allowing a higher tolerance in the production process of CIGS solar cells.

Acknowledgment

We thank Bas J. Kniknie (TNO) for the SEM image of the CIGS solar cell, as displayed in Fig. 1.