Modelling of Cu(In,Ga)Se₂ Solar Materials/Devices

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Abstract

This paper will present the numerical modelling of CIGS materials/devices in order to better understand the physical properties of the device, having the goal to support/improve the fabrication technology based on an alternative hybrid sputtering/evaporation deposition. Optimization of the buffer- and absorption layer for high efficiency CIGS solar cells will be presented, since the band gap can be graded over a wide range by changing the Ga concentration in the thin film layer, which greatly affects the efficiency of the solar cell. The dependence of the solar cell properties on the thickness of the buffer layer and the effects of the bulk and interfaces defects on the solar cell parameters have been studied.

The hybrid approach to modelling and simulation of thin film solar cells with a metal front grid on top of the transparent conductive oxide based electrode will be presented. A 3D model with high aspect ratio of device thickness (100s of nm) and its length and width (mm and cm range) was divided into two coupled models with different number of spatial dimensions (a 1D and a 3D model) on different length scales. The first one covers the modelling on the material stack level. The second model is coupled with the first and it takes into account the photovoltaic device's geometry. This approach enables the separation of the technology-dependent material simulation from the device shape and front grid design simulation. The metallization in the form of parallel fingers was investigated and optimized

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for the described case study. Finally, the efficiency of solar thin-film modules using optimized cells with different widths will be explored, thus enabling the tuning of the output voltage of the solar module while the power output remains unchanged.

Keywords: CIGS, thin-film, solar cells, modelling, simulation.

1 Introduction

Materials modelling, as well as device modelling, and the use of the developed models to simulate the materials/devices functionalities are indispensable in the improvement of the technology processes for all industries, including photovoltaic industry. Precise materials models enable much faster material development and decrease the number of needed expensive experimental steps to only those validated by the simulations first.

This paper presents numerical modelling of thin film photovoltaic materials/devices based on Cu(In,Ga)Se_2 (CIGS) technology in order to better understand the physical properties of the device, with a goal to support/improve the fabrication technology.

Among the thin-film technologies, solar cells based on CIGS absorber material are the most promising [1]. CIGS is a direct band gap semiconductor characterized by a high absorption coefficient [2]. Additionally, the band gap can be graded over a wide range by changing the concentration of gallium in the thin film absorber layer [3].

2 Modelling Strategy

Electrical modelling on the material level was performed using SCAPS-1D simulation software [4]. Current-voltage (I–V) and external quantum efficiency (EQE) curves are simulated and compared with experimental data. The numerical model was calibrated to the measured values of solar cell samples, based on the recently developed technology based on an alternative hybrid sputtering/evaporation deposition [5]. The baseline set of the parameters used for the simulations is obtained from the measurements performed on each separate layer of the samples and from a study of the data found in works of other authors [6–8]. The thicknesses of the individual layers were obtained from profilometer and scanning electron microscopy (SEM) measurements, and are the following: Mo(800 nm)/CIGS(1.8 μm)/CdS(50 nm)/ZnO

(100 nm)/ZnO:Al(330 nm). The Ga grading profile within the absorber layer was measured using secondary ion mass spectrometry (SIMS) [9].

In order to investigate the possibilities of size of solar devices (cells and modules), types of interconnection and front grid metallization, numerical simulations were carried out. The simulations were built upon the hybrid model of photovoltaic device, which consists of two coupled models: 1D material level model and 3D device level model [10]. The resulting I–V curve of the material simulation is used as an input data for the device based model. The diagram of the simulation steps with the input and output data is presented in Figure 1. The 3D model enables the simulation of devices with high aspect ratio thickness (100s of nm) and its length and width (mm and cm range). The photo-current flow through the transparent electrode is dictated by the shape of metal front grid. This approach enables the separation of the technology-dependent material simulation from the front grid design simulation. The device level model was done using COMSOL Multiphysics 4.2 simulation software [11].

The used devices are based upon the monolithically integrated cells within a module (serially connected cells with customizable size). The conductivity of the used transparent conductive oxide (TCO) is additionally improved using metallic front grid on top of TCO electrode. In this way the current collection capability of the device is improved, lowering the serial resistance of the device. However, the placement of opaque metallic grid introduces shading losses to the device, since less photons reach the absorber layer. Therefore, it is needed to make a compromise between electrical and optical losses, which can be done by simulation, using the proposed device model.

Figure 1 Flow diagram of the two-step hybrid simulation of CIGS material/device.

3 Simulation Results

The first stage model (material level model) is used to optimize technological properties of deposition of absorber (CIGS) and buffer (CdS) layer. The dependence of the solar cell properties on the thickness of the buffer layer (and absorption layer) and the effects of the bulk and interfaces defects on the solar cell parameters have been studied. Figure 2 shows the EQE curves of the simulated layers stack with the variation of thickness and defects density within the buffer layer. These variations have a large impact in the wavelength region of 300–500 nm. It can be seen that the thinnest buffer layer provides the best results, due to the reduced absorption, it enables more photons to reach the absorbing CIGS layer. However, the layers with density of several 10s of nm are hard to achieve in practice, resulting in non-uniform buffer layer which is not fully covering the absorber layer. Therefore, the optimum thickness value was found to be around 50 nm. The defect density, as expected, has a negative influence on the EQE in the same wavelength region.

Model of CIGS absorber layer includes the graded profile of gallium concentration along the layer thickness. The influence of Ga grading profile variation on the performance of the cell is presented in Figure 3. The grading data were collected both from the measurements (samples A, B, C) and from the literature [3]. Simulation results show the existence of correlation between Ga grading profile and the recombination processes. From the simulations it was observed that a too strong Ga grading profile increases the probability

Figure 2 Simulation of EQE (external quantum efficiency) of the device with variation of CdS buffer layer's: a) thickness, b) density of defects.

Figure 3 a) Variation of the Ga grading profile within the absorbing CIGS layer. b) Corresponding I–V curves.

for electrons to recombine, due to the formation of a barrier in the conduction band behind the space charge region [9]. However, the performances of the solar cells with different Ga profiles are not just influenced by the effects of this notch, but also the defects density is elevated at the areas of rapid Ga grading. It can be seen that the favourable grading has somewhat smaller concentration difference in the front and in the middle of the device, which results in the better I–V curve shape. Also, other critical properties of the absorber layer, such as thickness, defect density, conduction band offset between absorber and buffer layer, etc. are taken in the consideration, in order to properly optimize the parameters of the material deposition process.

After the simulation on the material level, the resulting I–V curve was used as an input for the simulation on the device level. In the following example, a solar cell with dimensions $1 \times 2 \text{ cm}^2$ (the cell interconnection line is on the shorter edge of the cell) was simulated in order to optimize the metallization on top of the TCO layer. The metallization was applied in the form of parallel fingers, orthogonal to the interconnection line (parallel to the longer edge of the cell). The metallization was assumed to be screen-printed, with lines $10 \mu\text{m}$ thick and $200 \mu\text{m}$ wide. The spacing between the metallization lines was varied from 1–10 mm. The resulting I–V curves of such a device are presented in Figure 4. Also the case when no metallization was applied is presented in the figure. The curve labelled “Perfect cell” presents the I–V curve from 1D model, with no electrical and optical losses caused by the front electrode (TCO + metallization). It can be calculated that the optimal distance is around 4 mm, with the minimum losses of 17% caused by shading and serial resistance.

Figure 4 a) Meshed geometry of the simulated device. b) Simulated I–V curves of a cell with added metallization in the form of parallel fingers with different spacing.

4 Conclusion

This paper presented the modelling strategy of thin-film solar cells using two loosely coupled models on material and device level. The presented method was also successfully used to simulate curved thin-film modules [12], with the addition on the scaling factor dependent on the device's geometry and the position of the illumination source.

The flexibility of the CIGS technology to produce modules of irregular shapes and sizes, enables the application of CIGS-based modules primarily in the field of product and building integrated photovoltaics (PiPV and BiPV). The presented numerical models were successfully used to simulate such unconventionally shaped thin-film solar modules [13].

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Biographies

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