Solar Energy Materials & Solar Cells ∎ (∎∎∎∎) ∎∎∎–∎∎∎

Contents lists available at ScienceDirect

Solar Energy Materials & Solar Cells

journal homepage: www.elsevier.com/locate/solmat

Approaches and challenges in optical modelling and simulation of thin-film solar cells

Marko Topič*, Martin Sever, Benjamin Lipovšek, Andrej Čampa, Janez Krč

University of Ljubljana, Faculty of Electrical Engineering, Trzaska 25, SI-1000 Ljubljana, Slovenia

A R T I C L E I N F O

Article history:
Received 7 June 2014
Received in revised form
16 September 2014
Accepted 18 September 2014

Keywords:
Solar cell
Optical modelling
Thin film

A B S T R A C T

Optical modelling and simulations present an indispensable tool in the design, analysis and optimisation of thin-film solar cells of different technologies. In this paper highlights and challenges of different numerical modelling approaches are reviewed, from one-dimensional to rigorous two- or three-dimensional optical modelling. A concept of Coupled Modelling Approach (CMA) is proposed to be used, in which different optical models are coupled together to achieve best performance in speed and accuracy of simulations. A Combined Ray-Optics Wave-optics Model (CROWM) is presented as a simple example of the CMA. In the second part two examples of modelling and simulations are presented. To demonstrate the applicability of 3-D rigorous optical modelling, results of optimisation of periodic substrate surface texture in a micromorph silicon solar cell are shown. Furthermore, a model of non-conformal layer growth is employed to determine morphologies of internal interfaces and to make a selection of suitable textures for defect-less thin-film silicon layer growth. The CROWM simulator was employed to demonstrate the usability of coupled modelling on the example of optimisation of macro-textures in organic solar cells.

1. Introduction

Performance of thin-film solar cells needs accelerated improvements. Apart from inevitable energy conversion losses, the origins of remaining electrical and optical losses need to be clearly identified for thin-film PV technologies and solutions for further improvements found.

In case of thin-film solar cells with indirect semiconductor absorbers (such as silicon), or cells based on direct semiconductors with very thin absorbers (such as thin CIGS or CdTe) or other thin-film technologies (organic and others), light management can still contribute to boost the conversion efficiencies of the devices. Reducing reflection at front interfaces, improvements in trapping of light, the reduction of optical losses in supporting layers and optimal distribution of light absorption in case of multi-junction devices are the key challenges to be focused on in solar cell optics. In this respect optical modelling and simulations play an important role in the design, analysis and optimisation process. By modelling we mean development of appropriate physical and numerical models, whereas simulations are mostly linked to using the models to calculate performances of devices. However, often term modelling is used for both. By modelling and simulations one has a complete insight in the optical phenomena, determining the external characteristics of devices. The same holds also for electrical modelling and simulations. On the other hand, modelling and simulations have a power to predict limits in performances of specific device concepts and indicate possible solutions to approach them. Furthermore, they enable fast and efficient optimisation of the devices, compared to experimental trials. Analytical methods are still important to define theoretical limits of light absorption in thin and thick layers of generalised structures, considering coherent and incoherent nature of light and isotropic or anisotropic light scattering [1–3]. However, numerical modelling supported by computer simulations enables detailed analysis of complex realistic structures [4].

In this paper we focus on numerical modelling of thin-film solar cells, addressing one- (1-D), two- (2-D) and three-dimensional (3-D) approaches. Main advantages, drawbacks and challenges are discussed in Section 2. Furthermore, a concept of a coupled modelling approach (CMA), combining different models into one unique model, is presented. In Section 3 two selected cases of applications of optical modelling are shown: (i) 3-D rigorous optical modelling of silicon micromorph solar cell, including a model of non-conformal layer growth and (ii) an example of coupled modelling approach, employing Combined Ray-Optics Wave-optics Model (CROWM) [5] for optimisation of organic solar cells. Nano- and macro-textures are optimised by means of 3-D optical models, for improved light trapping, in case (i) and (ii), respectively.

2. Numerical modelling approaches and challenges

2.1. An overview of modelling approaches

Nowadays, numerical modelling is widely used to predict, analyse and optimise the performances of PV devices. Thin-film solar cells

* Corresponding author.
E-mail address: Marko.Topic@fe.uni-lj.si (M. Topič).

http://dx.doi.org/10.1016/j.solmat.2014.09.026
0927-0248/

present relatively complex optical system since they consist of many layers (6–20), including nano- or macro-structures for efficient light trapping. The optical system usually includes thin and thick layers (in relation to effective wavelength of light), which requires both, coherent and incoherent treatment of light propagation in multilayer structures.

In next sub-sections we briefly present an overview and selected highlights of modelling approaches for simulation of thin-film solar cells. We decided to divide the approaches with respect of spatial dimensions considered in the model, in particular 1-D (Section 2.1.1) and 2-D and 3-D (Section 2.1.2).

Independently of the modelling approach taken, it has to be stressed already at this point that accurate input data (complex refractive indexes, layer thicknesses, scattering parameters in case of 1-D modelling, exact texture morphology and others) present a key pre-requisite for realistic simulations. Methods for determination of input parametrs can be found elsewhere [4,6].

2.1.1. 1-D optical modelling

Despite the fact that computer speed and power are boosting from year to year, there still exist advantages of 1-D optical modelling of thin-film solar cells, compared to 2-D or 3-D rigorous and other comprehensive modelling approaches. Usually 1-D simulations are very fast, also for complex structures that employ texturing features, which is especially important for extensive iterative optimisation or just for a quick conceptual testing of devices. The physics of multilayer optics and of light scattering process at nano-structures are important for building reliable models for thin-film solar cells [4]. 1-D models are essential for quantifying and understanding of optical effects happening inside the structures, since the theory and consequently the equations behind are still relatively simple. For instance, with certain level of accuracy we can clearly identify distribution of light absorption in multilayer semi-transparent structures, including the absorption in active layers and optical losses in the supporting layers. Disadvantages of 1-D modelling are mainly linked to approximations that have to be considered to represent realistic 3-D problem in 1-D space. In thin-film silicon solar cells one of the important issues still presents the approximation of light scattering at random nano-textured interfaces. Commonly, scalar scattering theory (SST) is used to determine light scattering at textured internal interfaces [7,8]. First it was applied to determine haze parameters of reflected and transmitted light at textured interface (amount of scattered light with respect to total (specular+scattered) reflected or transmitted light at an interface) [9–11]. Modifications were introduced to the original equations [12–14] to achieve a better level of approximation of wavelength dependent haze parameter outside the range of model validity (for textures with large root-mean-square roughness and lateral dimensions comparable to light wavelength in actual medium). Later on, SST was applied also to estimate angular dependency of scattered light inside the structure (angular distribution function) [15–17]. Thus, both descriptive scattering parameters, haze and angular distribution function, which carry key information on light scattering can be calculated for each textured interface in the solar cell structure. Some of 1-D models, such as Genpro 4 [18] enable refraction of light at macro-textures to be included in angular distribution function as well. Also plasmonic effects on metal nanoparticles have been incorporated in 1-D modelling [19].

Besides description of light scattering, coupling of coherent and incoherent propagation of light in thin-film structures was integrated in 1-D modells, such as in Sun*Shine* [11,20], Genpro 3 [21], Cell [10] and other models [18,22]. Coherent nature of light was assigned to specular light propagating in thin layers, which thicknesses are in the range of effective light wavelengths. Once the light is scattered at random nano-textured interfaces its coherency is assumed to be fully lost in the modelling and its propagation described by incoherent light beams also in thin layers. Such approximation results in an appropriate suppression of interference fringes in simulated spectral responses of thin-film devices, supported by good agreement with measured spectral characteristics [23].

In the past 1-D modelling and simulations have demonstrated also their predictive power in indicating realistic limitations in optical performances of thin-film solar cells [24] or predicting improvements related to specific effects, such as the effect of high haze parameter and broad angular distribution function of scattered light [25]. The importance of minimisation of optical losses was demonstrated and the role of different layers (materials) investigated. One of them was the research of suitable material for intermediate reflector in micromorph tandem cells. Besides commonly used ZnO transparent conductive oxide, alternative materials such as SiO_2 and MgF_2 were studied by 1-D simulations as reported in [26]. A few years later, SiO_x material became one of the most promising candidate for intermediate reflector indeed [27,28]. Other materials (e.g. MgF_2) in the role of interlayer are still under development [29].

2.1.2. 2-D and 3-D rigorous optical modelling approaches

In case of thin-film solar cells, 2-D and 3-D optical modelling was mainly introduced to consider light scattering and antireflection effects at (nano)structures, avoiding certain approximations used in 1-D modelling (such as SST and 1-D ray tracing). Here, the geometry of those structures is directly imported in simulations and linked to optical effects via Maxwell's equations. Recently, the computational power and speed of commercially available computers have come to the stage that realistic thin-film solar cells can be simulated using rigorous methods in 2-D and especially 3-D space. Different solving methods are used to resolve the optical situation in thin-film solar cells, among them are: Finite Element Method (FEM) [30], Finite Difference Time Domain (FDTD) [31], Finite Integrating Technique (FIT) [30], Rigorous Coupled Wave Analysis (RCWA) [32] and others. All of them have been successfully demonstrated for simulation of thin-film silicon solar cells, for example FEM in [33,34], FDTD in [35–39], FIT in [40,41], RCWA in [42,43] and others, like rigorous diffraction theory, in [44].

Selected simulation issues that need special attention when performing rigorous simulations are highlighted here. They mainly refer to the case of FEM, partially they can be extended to other methods too. First, appropriate spatial meshing of the simulation domain and setting the correct boundary conditions appear to be two of the most critical issues in accurate 2-D and 3-D rigorous optical simulations. With respect of boundary conditions (periodic, symmetrical, absorbing [30]) one has to pay special attention to the light which reaches the boundaries of the simulation domain under oblique angles. For example, 1st order Absorbing Boundary Condition (ABC)) is an appropriate choice for perpendicular incidence whereas for oblique angles it may lead to a significant error [30]. Therefore, in case of light scattering higher order ABC or perfectly matched layer (PML) boundary conditions are preferred to minimise unwanted reflections at the borders of the simulation domain. Furthermore, a sufficiently dense mesh is required (in the range of more than $5 \times 5 \times 5$ discrete points per effective wavelength cube in 3-D, for the first order of field approximation between two points) to avoid errors in calculations. Higher orders of field approximation (e.g. quadratic) between two points can further reduce the errors, but may increase the computation time significantly, according to our experiences. Furthermore, mixed order approaches in combination with appropriate unstructured meshing can commonly lead to a very good geometrical and physical problem adaptivity and a lower computational complexity than single order approaches. The dense meshing restrictions can be of vital importance for simulation of complete thin-film silicon solar cell, certainly if including, for

Please cite this article as: M. Topič, et al., Approaches and challenges in optical modelling and simulation of thin-film solar cells, Solar Energy Materials and Solar Cells (2014), http://dx.doi.org/10.1016/j.solmat.2014.09.026