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Modelling of thin-film silicon solar cells

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ABSTRACT

Computer modelling has become increasingly important in the design and optimization of surface textures that are used in thin-film solar cells to manipulate scattering of light. Light scattering at rough interfaces together with efficient back reflector is a standard approach to enhance absorption of light in the absorber layers of thin-film silicon solar cells. Substrates with randomly textured surface are commonly used to introduce rough interfaces into solar cells. Scalar scattering theory was used to describe light scattering at random nano-textured interfaces and to optimize random texture in single junction solar cells. Recently, substrates with periodic surface features have been investigated as an alternative to randomly surface-textured substrates. Three-dimensional Maxwell equation solvers were used to analyse and optimize such periodic textures when embedded in single and multi-junction solar cells. In both random and periodic cases, opto-electrical modelling was employed to assess the spectral response, to evaluate optical losses and to simulate current density–voltage characteristic.

1. Introduction

One of the major photovoltaic (PV) technologies for large-scale electricity generation is thin-film silicon PV technology. This technology utilizes solar cells based on thin absorber layers of hydrogenated amorphous or nano-crystalline silicon films and its alloys such as silicon–germanium. Thin-film silicon solar cells are characterised by short energy payback time and are fabricated with small amount of raw materials. Such properties make this technology attractive to the PV market.

However, the initial conversion efficiency of thin-film silicon solar cells has to achieve a level of 20% in order to stay competitive with bulk crystalline silicon solar cells and other thin-film solar cell technologies, such as those based on binary, ternary, and quaternary absorber compounds [1–5]. In general, both absorption of light in the absorber layers and collection of photo-generated charge carriers at the electrodes have to be further optimized in thin-film silicon solar cells. Therefore, light management is one of the key issues for improving the performance of thin-film silicon solar cells. Proper light management allows thickness reduction of the absorber layers, which means less material consumption and a decrease in production costs by shortening deposition times.

Light management aims to maximise the absorption solar energy radiation in the absorber layers. Light management is accomplished with a number of techniques that mainly focus on the following areas: (i) effective use of the solar spectrum by employing multi-junctions [6–11] or spectrum splitters [12–14]; (ii) minimization of absorption outside the absorber layers by implementing supporting layers-doped layers and transparent conductive oxides (TCOs)-with low parasitic absorption [15–18]; (iii) *trapping* of light inside the absorber layers. Light trapping techniques are an important part of light management. Their function is to couple light inside the solar cell, especially in the absorber layer(s). The following techniques are used to couple light inside the absorber layer:

- in-coupling of incident light at the front side [19–25];
- reflection at the back side [26–31];
- intermediate reflectors in multi-junction solar cells [32–35];
- light scattering at rough interfaces [36–41];
- light scattering using metal nano-particles (plasmonic effects) [42–50].

Two areas in the development of light trapping techniques can be distinguished. The first area manipulates the device reflectance. For this purpose, optically active layers are developed, such as anti-reflective coatings, single films or stack of layers for index matching, intermediate and back reflectors. These layers, designed from both material and thickness points of view, aim to decrease the total reflectance at air/solar device interface. As a result the amount of light that initially enters the absorber(s) is increased. The second area promotes light scattering. This is achieved by implementing nano-textured interfaces. Light scattering depends on the morphology of such interfaces, usually introduced into a solar cell through textured substrate carriers. Scattering at rough

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interfaces changes the incidence angle of electromagnetic field inside the absorber layers thus facilitating the coupling of light in the absorber layer(s). In addition, nano-textures have also an anti-reflective effect. Recently, layers of metal nano-particles and composite materials with embedded metal nano-particles designed for efficient in-coupling and scattering of light into the absorber layer have been demonstrated [50].

Standard light trapping techniques in today's thin-film silicon solar cells are based on scattering of light at randomly textured rough interfaces, the employment of highly reflective metal layers at the back contact and refractive-index matching layers at the front side. The rough interfaces are introduced into solar cells by using substrate carriers that are coated with TCO layers with nano-textured surfaces, such as fluorine-doped tin oxide (FTO) of Asahi U-type substrate with a pyramidal-like surface structure [36] and sputtered aluminium-doped zinc oxide (AZO) that after etching in a 0.5% hydrochloric acid solution shows a crater-like surface texture [37].

By combining geometrical ray optics with statistical mechanics, Yablonovitch calculated the theoretical potential of using nano-textures in solar cells [51]. He showed that the absorption in a slab with nano-textured surfaces, which is bathed in blackbody radiation and confined with a white reflector on one side, is increased by a factor of $4n^2$, where n is the refractive index of the absorber material. Another way to look at the potential of nano-textures is in terms of number of ideal passes (NIP). Ideally, the absorption due to light coupling in a textured slab thick d can be numerically seen as the standard 2-passes absorption of light [52] in an equivalent flat slab. The thickness of such equivalent flat slab is $\text{NIP}\cdot d$ and is called *effective optical thickness*. Fig. 1 shows the results of a recent study of the impact of effective optical thickness on the photocurrent of thin-film silicon solar cells carried out by Zeman et al. [53]. They used advanced computer programs in their study such as the Advanced Semiconductor Analysis (ASA) program from Delft University of Technology [54] and the Sunshine program from Ljubljana University [55]. Their results are presented in Fig. 1 and demonstrate that multiplying a 300 nm thick slab of hydrogenated amorphous silicon (a-Si:H) and a 1 μm hydrogenated nano-crystalline silicon (nc-Si:H) by NIP=10 increases the absorption of sunlight by 52% and 90%, respectively. Multiplying the same geometrical thicknesses by NIP=50 leads to an increase in absorption of 78% and 138%, respectively. The results of Yablonovitch and Zeman et al. demonstrate the importance of scattering at nano-textures for enhancing the performance of thin-film silicon solar cells. The scattering properties of various materials with different nano-textured surface morphologies have been extensively studied in the last decades. The studies are aimed to develop nano-textures that maximise the absorption in the absorber layer. To carry out such optimization experimentally is a very cumbersome task. Modelling has proven to be a powerful method to study the effect of nano-textured interfaces on the performance of thin-film silicon solar cells [56,57]. Moreover, modelling is also a powerful mean to design optimized nano-textures for obtaining maximal absorption in the absorber layer resulting in a high photocurrent.

This paper presents an overview of opto-electrical models developed at Delft University of Technology for thin-film silicon solar cells on random (see Section 2) and periodic (Section 3) textured interfaces: (i) opto-electrical modelling of single junction solar cells based on random textures using Fast Fourier Transform, annealing algorithm and semiconductor equations solver; (ii) three-dimensional (3-D) optical modelling of single junction solar cells on periodic gratings in the hypotheses of conformal growth using Finite Element Method in frequency domain; (iii) two-dimensional (2-D) optical modelling of single junction solar cells on periodic gratings in the hypotheses of non-conformal growth using Finite Difference Time Domain method; (iv) hybrid opto-electrical modelling of triple junction solar cells on periodic gratings in the hypotheses of conformal growth using Finite Element Method in frequency domain and semiconductor equations solver.

2. A scalar scattering model

To describe scattering of light at nano-textured interfaces in the far field, as illustrated in Fig. 2, usually two descriptive scattering parameters are used. First is the angular intensity distribution [AID, also called angle resolved scattering (ARS) or angular distribution function (ADF)] that indicates how much light of a certain wavelength is scattered into a certain angle. Second is the haze that is an integrated parameter and is defined as the fraction of the light which is scattered. Both the AID and the haze can be defined in transmission and reflection.

In the last years three models were published that can predict the AID and/or the haze in transmission [58–60]. All three models use the height function $z(x,y)$, indicated in Fig. 2, of the nano-texture as input and are based on the fact that in the first order the scattering object and the scattered field are related to each other via Fourier transforms. Recently the three models were re-evaluated and improved such that a full scattering model is available that can calculate AID and haze in transmission and reflection for interfaces between arbitrary materials [61]. In this section the theoretical foundations of the scattering model are presented. After demonstrating the viability of the model to calculate the descriptive scattering parameters of different surface-textured materials, the model is applied for simulating complete thin-film silicon solar cells and used for investigating optimized interface morphologies.

2.1. The scattering model

In the scalar scattering theory, light is described as a complex scalar field $U(\mathbf{r})$ instead of the electromagnetic fields $\mathbf{E}(\mathbf{r})$ and $\mathbf{B}(\mathbf{r})$ [62]. The field in k-space is given by the Fourier transform of the pupil functions G_T and G_R, which contain the information about the nano-texture [58,59,64]:

$$U_T(K_x,K_y)=\frac{1}{2\pi}\iint_{\Re^2}G_T(x,y)e^{-i(K_x x+K_y y)}\,dx\,dy,$$
$$U_R(K_x,K_y)=\frac{1}{2\pi}\iint_{\Re^2}G_R(x,y)e^{-i(K_x x+K_y y)}\,dx\,dy, \tag{1}$$

where the subscripts T and R denote transmittance and reflectance, respectively. The geometry is indicated in Fig. 2. G_T and G_R are given by

$$G_T(x,y)=\sqrt{\frac{T}{A}}\exp\left[ik_0 z(x,y)(n_1-n_2)\right],$$
$$G_R(x,y)=\sqrt{\frac{R}{A}}\exp\left[ik_0 z(x,y)2n_1\right] \tag{2}$$

if (x,y) is inside the aperture of area A and $G_{T,R}\equiv 0$ elsewhere. Here, $k_0=2\pi/\lambda_0$ denotes the wavenumber *in vacuo*, λ_0 is the wavelength, and n_1 and n_2 are the refractive indices of the two materials that form the interface. The light is incident on the rough interface from the material with n_1. The morphology of the interface is contained in the height function $z(x,y)$. The constants $(T/A)^{1/2}$ and $(R/A)^{1/2}$ are chosen such that the total amount of light flowing through the aperture is equal to the total transmittance T or the total reflectance R of the interface, respectively. While in G_T both refractive indices are present in the exponent, in G_R only n_1 is present in the exponent. The latter indicates that the shape of the AID_R is independent of n_2, while its magnitude is controlled by R. Different possibilities for G_T were discussed in literature in the last years [58–60]. The Plancherel theorem intrinsically ensures energy

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