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Optical Simulation of Silicon Thin-Film Solar Cells

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Abstract

Efficient light trapping is essential for silicon thin-film solar cells. Excellent light trapping for silicon thin-film solar cells is achieved with randomly textured superstrates (TCO and/or glass). Due to a continuous and broad variation of occurring structure sizes in such textures, their optical simulation is challenging. In this paper we introduce an approach to establish a methodology for 3D optical simulation of silicon thin-film solar cells on randomly textured superstrates. The approach includes three steps. In a first step a fabricated structure is analysed to identify its typical geometric features. In a second step the single geometrical features are optically simulated using the rigorous coupled wave analysis (RCWA). The third step includes an investigation of how the results of the single features can be combined to describe the optical characteristics of the complete random structure. In this paper we concentrate on the first two steps. We introduce the analysis of an exemplary superstrate structure and investigate the optical properties of the single structure features. Preliminary results of this investigation are shown and a proposition of how to optimise the structure geometry is presented.

Keywords: Diffractive optics; simulation; textured superstrates; thin-film silicon solar cells

1. Introduction

Light trapping is an important feature to increase the absorption in solar cells. Light trapping aims to prolong the internal path of light inside a solar cell by increasing the probability for a photon to be

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absorbed and therefore contribute to current generation. Hence, light trapping can either be used to increase the cells' current or to reduce the actual thickness of the absorber layer. Both features are of key importance for silicon thin-film solar cells. Light trapping is typically realised by introducing a structure at one or both solar cell surfaces. Depending on the characteristics of the structure, its light trapping capabilities can be assigned to different physical effects. In silicon wafer solar cells one typical structure are pyramids on the front surface [1]. These pyramids have structure sizes of a few μm to up to 20 μm and they increase the optical pathlength by refracting light at the tilted surface. Considering that a fraction of the light is also trapped by total internal reflection, a considerable pathlength enhancement can be achieved by these pyramids. In addition, they also contribute to reducing front surface reflection losses by providing two or more interactions of a light beam with the surface. Using structure sizes in the sub 1-μm range, wave optical effects become more important. Depending on whether the structures are periodic or non-periodic, the dominant effects are either diffraction or incoherent scattering.

Incoherent scattering describes the process of redistributing light into the complete hemisphere. An ideal scattering surface shows a cosine distribution of the scattered light intensity. Such a characteristic is called Lambertian scattering. Scattering is typically used for light trapping in thin-film solar cells [2]. The maximum pathlength enhancement that can be achieved with scattering is given by the Yablonovitch factor $4n^2$, where n is the refractive index of the solar cell bulk material [3]. For silicon with $n \gg 3.5$, scattering results in a maximum pathlength enhancement factor of 50. This maximum is achieved, for example, for Lambertian scattering. However, realised structures often show much lower pathlength enhancement factors [4].

Even higher pathlength enhancement factors can be achieved with periodic structures and diffraction (sometime also referred to as coherent scattering). Diffraction describes the process of changing the direction of the incident light into several, diffracted directions. The basic idea is here to redistribute light into a direction alongside the cell, so that it stays in the absorber as long as possible. A theoretical limit of a factor of 3000 for silicon has been calculated by Kirchartz [5]. Efficient pathlength enhancement exceeding the Yablonovitch factor has been demonstrated for diffractive structures on several occasions (e.g. [6, 7]). However, diffractive effects are typically restricted to a very limited spectral range, while scattering can affect the complete spectrum. Experimentally, incoherent scattering has so far shown the better results.

In this paper we present a method to simulate light trapping structures for use in thin-film solar cells. The presented method is based on an approach developed for the simulation of diffractive structures in silicon wafer solar cells [8]. It can be divided into three steps: In the first step, a fabricated random structure that serves as the superstrate for the solar cell is analysed and typical geometrical structure features are identified. For this purpose we use the Generalised Hough Transformation (GHT) [9], an algorithm for detection of geometrical features in pictures. We use this algorithm to automatically detect and reproduce these features from atomic force microscope (AFM) measurements. In the second step, the single feature is simulated using the rigorous coupled wave analysis (RCWA) [10, 11]. RCWA is a tool that can be used for the optical simulation of diffractive structures. Using this tool, the most efficient structure features for light trapping can be identified. It must be noted, however, that the RCWA uses periodic boundary conditions. Thus, the performance of a periodic structure is calculated, rather than the performance of a single feature. In the third step the results for different features are combined to obtain the optical characteristics of the entire structure. The investigations related to the third step are not yet finalised; thus, the present paper focuses on the first two steps.

The texture investigated in this work consists of a ZnO layer sputtered on glass and wet-chemically etched in HCl. An AFM image of this texture is shown in Fig. 1. In first, simple simulations it is assumed that this structure acts as a superstrate onto which a layer of crystalline silicon with a constant thickness of 1 μm has been deposited. When deposited onto the ZnO substrate, silicon forms a conformal layer and is therefore also textured. The superstrate is assumed to have a constant refractive index of n = 1.5 (corresponding to glass). In this early stage, more accurate features (such as the exact solar cell structure including the refractive index and absorption of ZnO or a back surface reflector) are not yet included. A refinement of the method including these features is currently in progress.

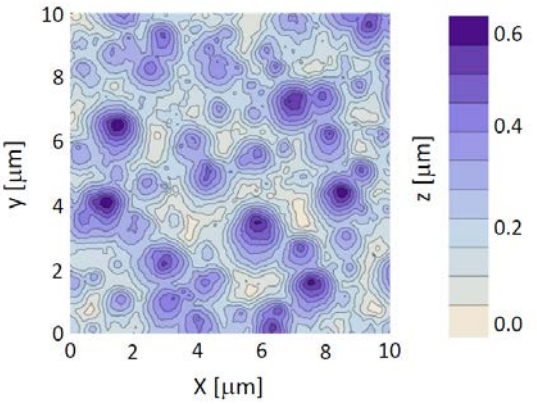


Fig. 1. Contour plot of an AFM measurement of the investigated structure. The structure was produced on glass by sputtering of ZnO and subsequent wet-chemical etching in HCl.

In the next section we give a short introduction into the RCWA and the approach to detect typical geometrical structure features. We show results of an investigation of the light trapping capabilities of the single features. Finally, we show first results for the complete structures based on a superposition of reflection and transmission data.

2. Simulation methods

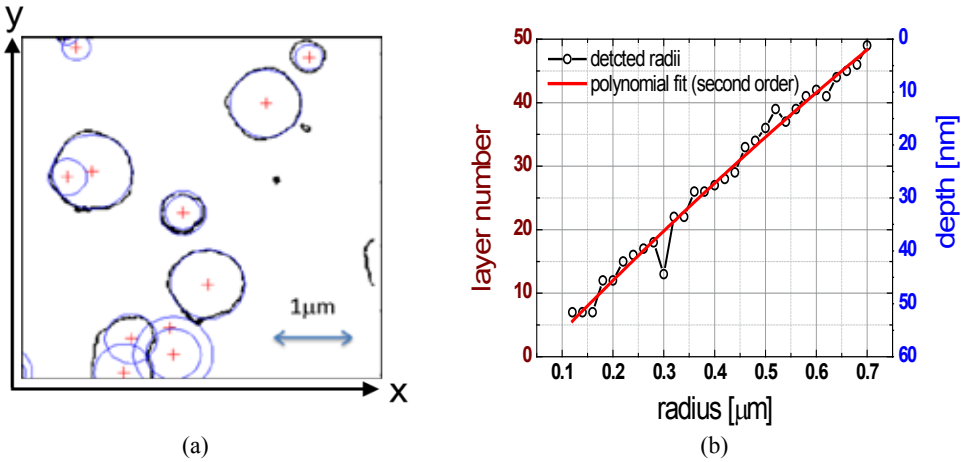
2.1. Rigorous coupled wave analysis (RCWA)

To perform wave optical simulations, we used a Matlab-based RCWA code [10] written by Lalanne *et al*. [11]. In this method, a structure is divided into several layers. The refractive index in each layer is represented by a step function. The step function is decomposed into a Fourier series. This procedure implies the use of periodic boundary conditions; RCWA therefore is basically designed to model periodic structures. Additionally, the electric field in the different regions (superstrate, structure, and substrate) is also decomposed into a Fourier series. Each Fourier component corresponds to a plane wave that can be identified with a diffraction order. The electromagnetic field is solved mode-wise in each layer. Finally, the layers are re-assembled and the boundary conditions are matched to obtain the solution for the complete structure.

The method allows calculating the electromagnetic near- and far-field inside and outside the solar cell. This includes the spectrally and spatially resolved reflection, transmission and absorption spatially resolved, mode-wise as well as integrated.

2.2. Detection of typical structure features using the Generalised Hough Transformation (GHT)

To analyse and auto-detect the geometrical features, we developed a method based on the Generalised Hough Transformation (GHT). The implementation used for this purpose was written by Peng in Matlab [12]. The GHT allows detecting circles in a picture. The detection includes the position and the radius of the circles. Since for the RCWA simulation the structure is divided into layers, the approach followed was to divide the measured AFM data into layers or cross sections. These cross sections were represented in pictures and the GHT was then used to detect circles in the cross section. The result of an exemplary part of one of these cross sections is shown in Fig. 2(a). As can be seen, features that are sufficiently circular are correctly detected by the method; however certain artefacts remain so that in some places circles are detected that don't actually exist. To ensure that these artefacts are not incorrectly detected as features, the centre positions of the circles are cross-linked to the positions of minima on the structure. For each of the detected features, the radius is recorded in the different layers. Knowing the radii in the different layers, the geometrical form of a feature can be reconstructed, see Fig. 2(b). In this way, more than ten typical structures have been identified on the investigated sample.



(a) (b)

Fig. 2. (a) Circle detection using the GHT in a single layer. The actual structure is coloured black; the blue circles are closest fits using the GHT. The red crosses show the circle centres. For a clearer picture, only a fraction of Fig. 1 is shown. (b) Reproduction of the radii in different layers to obtain the geometrical structure for one structure element. The red line is a second-order polynomial fit. The etching process creates craters. For most of the found craters, the radius shows an almost linear dependence on the depth.

It has to be said that the presented approach currently only works if the investigated features are sufficiently circular. Geometries deviating from circular shape - like ellipses or more complex forms - can currently not yet be detected. However, with an adapted version of the GHT, this will be possible.

3. Simulation results

3.1. Absorbed photocurrent density

To quantify the performance of each structure element, the absorbed photocurrent density j_{ph} was calculated. For this calculation a square unit cell was assumed, the diagonal of which is twice the maximum radius found for a given structure. In that way, no planar surfaces occur. j_{ph} is given by

$$j_{ph} = q \int_{\lambda_{min}}^{\lambda_{max}} N_{AM1.5}(\lambda) \cdot a(\lambda)\ d\lambda \qquad (1)$$

In this equation q is the elementary charge, $N_{AM1.5}(\lambda)$ is the density of photons in the AM1.5 spectrum and $\alpha(\lambda)$ is the wavelength dependent absorption. λ_{min} and λ_{max} mark the lower and upper boundary of the spectral range considered. In the simulations performed in this work, we used the spectral range from λ_{min} = 600 nm to λ_{max} = 900 nm, as in this spectral range the penetration depth of light into silicon considerably exceeds the used absorber layer thickness yet still a significant fraction of the incident light is absorbed. The photocurrent density in the solar spectrum, i.e. the current density that a solar cell would produce if every photon was absorbed, in this range is $j_{ph,max}$ = 19 mA/cm^2.

Figure 3 shows the calculated j_{ph} for ten identified typical structures. Also shown, as a reference (red line), is the calculated absorbed photocurrent density for a planar absorber layer ($j_{ph,ref}$ = 3.16 mA/cm^2). Since the reference constitutes the case in which the light takes the shortest possible path, it is not surprising that every textured structure yields a higher j_{ph} than the reference; however, many of the structures only result in a slightly better performance. Yet some structures result in an up to more than threefold increase in the number of absorbed photons (#9 and #10) and therefore very efficient light trapping. Note that the simulation assumes periodic boundary conditions; the features are arranged in a quadratic pattern that is infinitely extended in the x and y direction. The calculated light trapping induced by these structures is therefore partially induced by diffraction. At this point it is not yet clear how the results for the single features can be used to reproduce the results of the whole structure. The approach we want to follow is to use a superposition. The simplest superposition is to use the average of the calculated photocurrent to simulate the absorption induced by the random structure. If this approach is valid then the proposed method allows identifying parameters for a periodic structure that can improve the performance of the structure. Looking at the geometrical features of the simulated structures, the common feature of structure #9 and #10 is that they are the smallest of the investigated structures. The sizes of the identified structures vary between 0.65 µm and 1.6 µm (see Table 1). The results indicate that smaller structure sizes are generally preferable over larger sizes. The best result, however, is obtained for a structure with a size of 0.77 µm, which suggests the existence of an optimal structure size. The optimum will be identified in the course of on-going investigations.

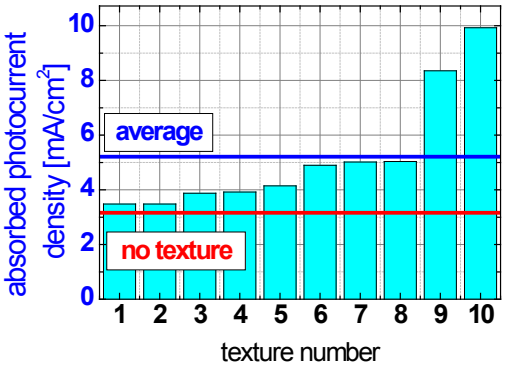


Fig. 3. Calculated j_{ph} values obtained from an optical simulation with RCWA for the ten different identified structure features. Note that RCWA assumes that the structures are periodic in two dimensions. Also given is the calculated j_{ph} for an absorber without structure (red line) and the average over all structures (blue line).

Table 1. Size and calculated absorbed photocurrent density for each of the ten investigated structures.

Number	*1*	*2*	*3*	*4*	*5*	*6*	*7*	*8*	*9*	*10*	*aver*	*ref*
Size (μm)	1.65	1.60	1.34	1.38	1.61	1.12	1.09	1.22	0.65	0.77	-	-
j_{ph} (mAcm^{-2})	3.48	3.48	3.87	3.92	4.15	4.89	5.02	5.03	8.35	9.93	5.21	3.16

In a next step we want to obtain information about the absorption in the non-periodic structure that is composed of the investigated single structures. The approach intended here is to calculate the electric field inside the structures in a first step and to perform a superposition of the electric fields. However, this calculation is still on-going. A very simple approximation to get a first idea of the performance of a random structure is to superpose the simulated absorption spectra. The result of this simple estimation is shown as the blue line in Fig. 3. The corresponding absorption profile is shown in Fig. 4. Also shown there is the absorption profile calculated for the reference. The reference clearly shows Fabry-Perot oscillations as features of interference effects. The calculated averaged absorption profile shows only little oscillations, which indicates that already in this simple approach most of the interference effects are eliminated, which would be expected for a scattering surface.

Finally, we calculated the absorption also for a Lambertian scattering surface in the cell. This calculation was performed by using a planar setup and increasing the thickness of the absorber by a factor of 50 ($4n^2$). In this case we obtained an absorbed photocurrent density of $j_{ph} = 15.25$ mA/cm^2.

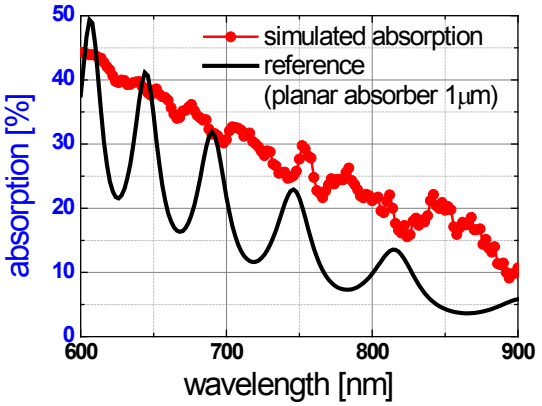


Fig. 4. Calculated absorption profile for the average of all structures and for the reference. The absorption profile is the average of the absorptions calculated for the single structure features.

3.2. Pathlength improvement

To analyse the quality of the light trapping provided by the structures we calculated the pathlength improvement factors for the different structures and for the average. A derivation of the pathlength improvement factors can be found in Ref. [13]. In the approach described there, a solar cell with a back surface reflector is analysed. Since no such reflector is applied in our present study and therefore a fraction of the light is transmitted, the method must be adapted. In the used approach it is assumed that most of the reflected light is reflected when the light impinges on silicon for the first time and that most of the non-absorbed light is transmitted through the system. The equation to calculate the pathlength improvement factor on the absorption κ_a is then given by

$$\kappa_a = \frac{ln\left(\frac{T(\lambda)}{1-R(\lambda)}\right)}{ln\left(\frac{T_{Ref}(\lambda)}{1-R_{Ref}(\lambda)}\right)} \quad (2)$$

In this equation $R(\lambda)$ is the spectrally dependent simulated reflection and $T(\lambda)$ the transmission. The index *Ref* indicates values for the reference. The result of this analysis is shown in Fig. 5. In this graph we show the pathlength improvement calculated for the structure for which the highest current (#10, green line) and the lowest current (#1, red line) is obtained. Also calculated is the improvement for the average of all investigated structures (blue circles). With the best structure, the pathlength is increased by up to a factor of ten compared to the reference. Note that the reference also includes a certain amount of light trapping and that this simple approach does not correctly account for light escaping through the front surface after the first reflection at the rear. This results in an underestimation of the actual pathlength enhancement with respect to values typically found in the literature. To illustrate this underestimation, we have calculated the pathlength enhancement with this equation also for a Lambertian scatterer. For this case we would have expected the theoretically possible values in the range of 50, however, due to the above-mentioned reasons, the calculated enhancement was only about 35. This underestimation also explains why for the "worst" structure (red line) values below one are possible. However, it needs to be said that the values below unity are to a certain extent also caused by oscillations due to coherent effects.

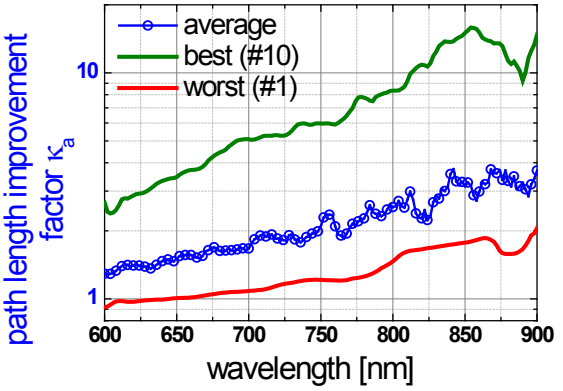


Fig. 5. Calculated pathlength improvement factors for the best structure (#10, green line), the worst structure (#1, red line) and the average over all structures (blue circles).

4. Summary

In summary, we have developed a method for the simulation of the optical properties of a 3D scattering structure for solar cell applications. The presented method follows a three step approach. In the first step, the structure is analysed and typical structure features are detected using the Generalised Hough Transformation (GHT). In the second step the single structure features are reconstructed and simulated using the rigorous coupled wave analysis (RCWA). In the third step the result obtained from the simulation of the single features are superimposed to reconstruct the optical properties of the entire structure. This third step is still under investigation and the paper concentrated on the first two steps.

The presented method was used to investigate and simulate an exemplary structure that consisted of sputtered and wet chemically etched ZnO on glass. The structure analysis was performed on an AFM measurement of this structure. On a sample size of 10×10 μm^2, ten single structure features were identified. The features mainly had the form of circular craters. The optical properties of a periodic array these craters were simulated using RCWA. The results of this simulation indicate that an optimum size for crater diameter exists. According to the simulations, this optimum is in the range of 700 nm, corresponding to the smallest of the investigated structures. It must be noted though that RCWA assumes periodic boundary conditions, adding a diffractive component to the results. How much this diffractive component affects the results is yet unclear. A first attempt to simulate the entire random structure with this method (step 3) was made by averaging the obtained results for the single structure features. However, for a thorough analysis the used model must be refined and compared to experimental results. Future steps will also include an analysis of the electric field inside the structure. Finally, we compared the obtained results to those obtained for an assumed ideal Lambertian scattering in the solar cell. We found that even the best feature of the investigated structure shows light trapping that inferior to the one induced by the Lambertian scattering.

Further development of the method will include a refinement and calibration with experimental input data and results. Eventually, the goal is to investigate many different structures and to identify the features that appear most promising for light trapping in thin-film solar cells. Identifying these promising features can help to optimise the texturing process and so realise optimum light trapping structures.

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