## 3D OPTICAL SIMULATION OF SCATTERING IN THIN FILM SILICON SOLAR CELLS

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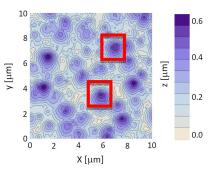
ABSTRACT: Efficient light trapping is of great importance for thin-film silicon solar cells. Randomly textured TCO or glass substrates provide excellent light trapping and are frequently applied. Optical simulation of such textures is challenging due to a large variety of occurring geometrical features. In this paper we suggest an approach for the 3D optical simulation of scattering structures. This approach is based on a simulation and investigation of the constituting single structure features and subsequent implementation of the solar cell structure into the rigorous coupled wave analysis (RCWA). In this paper we present first results of this method for a microcrystalline silicon solar cell deposited on a sputtered and etched ZnO surface. The simulated absorption for the single structures is compared to quantum efficiency measurements on large areas. Good agreement between simulation and measurement is found. Comparing periodic and random structures, we find that small periodic structures can increase the absorbed photocurrent density by up to  $3\text{mA/cm}^2$ . The best result was obtained for a structure with a diameter of D= 800 nm. Keywords: Diffractive optics; simulation; textured superstrates; thin-film silicon solar cells

# 1 INTRODUCTION

Light trapping is important to increase the absorption in solar cells. The goal of light trapping is to extend the internal path of light inside a solar cell. In that way the chance of contributing to current generation is enhanced. This enhancement is of particular importance for thin-film silicon solar cells. One way to realize light trapping here is by introducing a scattering structure at one or both solar cell surfaces [1-4].

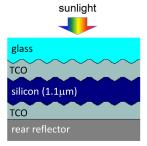
Incoherent scattering describes the process of randomly distributing light into a certain angular distribution. An ideal scattering surface shows a Lambertian characteristic, i. e. a cosine distribution of the scattered light intensity. The maximum pathlength enhancement that can be achieved with Lambertian scattering is given by the Yablonovitch factor  $4n^2$ , where *n* is the refractive index of the solar cell bulk material [5]. For silicon with *n*  $\square$  3.5, scattering results in a maximum pathlength enhancement factor of 49.

In this paper we suggest a method to simulate light trapping in a microcrystalline silicon solar cell. For this purpose a fabricated random structure that serves as the superstrate for the solar cell is analysed and typical geometrical structure features are identified. An AFM profile of the used texture is shown in Figure 1.Single geometrical features from this profile (red squares) haven been identified using the Generalised Hough Transformation (GHT) [6]. Following the identification of the single features, the solar cell is constructed and simulated using the rigorous coupled wave analysis (RCWA) [7,8] to determine the optical characteristics. A cross-section of the simulated setup is shown in Figure 2. The results of the single



**Figure 1:** AFM profile of a ZnO surface textured by a sputtering and etching process. The texture features circular craters with varying diameters in the mm and sub mm range. The red squares mark two single structure features that have been identified and investigated

features were compared among each other to find an optimum feature size. The single feature results were also compared to experimentally measured quantum efficiency data for a textured and a planar solar cell to validate and verify the method.



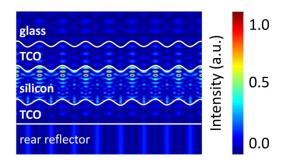
**Figure 2:** Sketch of the simulated structure (not to scale). The refractive indices for the materials are n = 1.5 for glass, n = 2 for TCO. For microcrystalline silicon, values measured at IMT were used. The rear reflector is an ideal mirror (n = 100000). The period corresponds to the single feature diameter *D*. For the investigated structure, the diameter was between  $D = 0.7 \mu m$  and  $D = 1.6 \mu m$ .

### 2 SIMULATION METHOD

### 2.1 Rigorous Coupled Wave Analysis (RCWA)

Wave Optical simulations have been performed using an implementation of the RCWA method in Matlab by Lalanne [8]. The investigated structure is divided into layers. In each layer the refractive index is considered to be a step function. Subsequently both the electromagnetic field and the refractive index function are decomposed into a Fourier series. This procedure corresponds to a decomposition of the EM filed into plane waves. Reordering the summands, the EM field in each layer can be solved mode-wise. Finally the layers are stacked and the boundary conditions between the layers are matched to obtain the solution in the whole structure. This procedure allows calculating optical near- and far field properties like reflection transmission and absorption. The result of a calculation of the EM field is shown in Figure 3.

The Fourier decomposition in the RCWA implies periodic boundary conditions. These conditions add diffractive elements to the calculated characteristics that do not occur in a random structure. Variations of the structure diameter and averaging processes are used to eliminate these effects. Details of this procedure are, however, not reported here.



**Figure 3:** Simulated intensity of the x-component of the magnetic field inside the structure calculated with RCWA for a wavelength of  $\lambda = 800$  nm. The magnetic field was used to illustrate the spatial distribution of the absorption. The calculated electromagnetic field is used to calculate the optical near- and farfield properties like reflection, transmission and absorption.

# 2.2 Structure Analysis

To analyse the geometrical characteristics of the single structures, a method for automatic structure detection was developed. This method is based on the Generalised Hough Transformation (GHT) and an implementation by Peng in Matlab [9] was used for this purpose. The basis for this analysis is the AFM profile shown in Figure 1. GHT allows detecting the central position and the radii of circles in a picture. This procedure has been used to

identify the diameter of the circles in each layer used for the RCWA simulation. The approach correctly reproduces the geometry of the craters.

### 3 RESULTS

#### 3.1 Performance of the single structure features

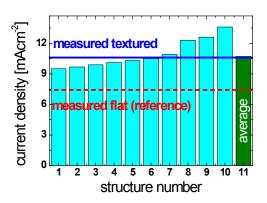
Knowing the absorption of the single feature, the absorbed photocurrent density  $j_{ph}$  was calculated by

$$j_{ph} = q \int_{\lambda_{min}}^{\lambda_{min}} N_{Am1.5}(\lambda) \cdot a(\lambda) \ d\lambda \qquad (1)$$

For the investigated solar cell with a thickness of  $1.1 \mu m$ , light trapping becomes important at around  $\lambda_{min} = 600 \text{ nm}$  and only very little light is absorbed above  $\lambda_{max} = 900 \text{ nm}$ . Note that all shown currents are given with respect to this spectral range. The results of the RCWA simulation for the single structure features are shown in Figure 4 (cyan bars). The structures have been ordered according to an increasing current. Also shown is the average for all structures (green bar) and the short circuit current density  $j_{SC}$  obtained for a planar sample (red dotted line) and a textured sample (blue solid line) .  $j_{SC}$  was calculated by

$$j_{SC} = q \int_{\lambda_{min}}^{\lambda_{min}} N_{Am1.5}(\lambda) \cdot EQE(\lambda) \, d\lambda \quad (2)$$

with the same values for  $\lambda_{min}$  and  $\lambda_{max}$  as mentioned before.



**Figure 4:** Absorbed photocurrent density for ten different single structures (cyan bars). Also shown is the average (green bar) and experimental results for a planar (red line) sample. The currents are calculated for a wavelength range between  $\lambda = 600$  nm and  $\lambda = 900$  nm.

structure	1	2	3	4	5	6	7	8	9	10	ref	av	exp
j <sub>ph</sub> / j <sub>SC</sub> [mAcm <sup>-2</sup> ]	8.7	8.9	9.7	9.9	10.1	10.5	10.9	12.3	12.6	13.6	7.4	10.9	10.6
diameter [µm]	1.6	1.2	1.6	1.7	1.4	1.1	1.3	0.7	1.1	0.8			

 Table 1: Summary of the results shown in Figure 4. Also given is the diameter of the single structure features for comparison.

The investigated samples were produced at the institute of microengineering (IMT), at the École Polytechnique Federale de Lausanne (EPFL). The structure was similar to that shown in Figure 2 with a thickness of the microcrystalline silicon layer of  $1.1\mu$ m. Potential sources of error are differences between simulated setup and the measured sample in the implementation of the TCO layer. In the simulation, absorption in the TCO layer was omitted. However, only very little absorption is expected in the TCO in the spectral range above 600 nm. Furthermore the exact thickness of the TCO was not known at the moment of the implementation. A quick check showed, however, that the effect of the TCO thickness is very small.

Comparing simulated and measured results we find that the average absorbed photocurrent density of the ten simulated structures  $(j_{ph,aver} = 10.9 \text{ mA/cm}^2)$  is very close to the measured short circuit current density  $(j_{SC}=10.6 \text{ mA/cm}^2)$ . Since the absorbed photocurrent neglects losses due to an imperfect collection it is also expected that  $j_{ph}$  should be higher than  $j_{SC}$ . This result is a first indication that the suggested method can be used to simulate random structures. However, to build up confidence and further investigate the method, more results are needed.

Looking at the detailed results for the single structure features, we find that each of them provides a considerable light trapping. Measurements for an untextured surface yield a current density of  $j_{SC} = 7.4 \text{ mA/cm}^2$ . The simulated absorbed photocurrent density varies between of  $j_{ph} = 8.9 \text{ mA/cm}^2$  of  $j_{ph} = 13.6 \text{ mA/cm}^2$  depending on the geometrical properties of the single structure features.

Provided that the assumption of averaging of periodic structures is a valid description for a random structure, there will always be single structure features that perform better and others that will perform worse than the average. The presented method allows identifying those features that perform best. In the presented example, structure number 10 results in a photocurrent density that is  $3\text{mA/cm}^2$  higher than the measured value. It can therefore be assumed that a defined periodic structure with the parameters given by structure number 10 can improve the solar cell efficiency considerably.

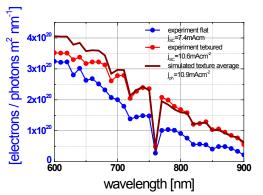
Finally we performed first investigation regarding influence of geometrical the characteristics of the single structure features on the solar cell performance. In Table 1 we compare the simulated  $j_{ph}$  with the diameter of the single structure feature. Since the features differ not only in parameter but also in form, this investigation is not unique. Still, a certain trend can be observed, which indicates that smaller structure sizes are preferable. The best result is obtained for a structure diameter of D = 800 nm.

A further important parameter is the aspect ratio of the structure, the ratio of diameter to depth. For this parameter, no consistent trend was found. Most structure features show, due to the etching process, similar shapes and therefore have similar aspect ratios. However, some of the identified shapes have aspect ratios that are significantly larger or smaller. From the existing dataset of ten points, no decisive conclusions could be drawn and a correspondence to the generated current could not be found. An investigation of the influence of the aspect ratio is carried out at the moment.

### 3.2 Spectral dependence of carrier generation

A more detailed picture of the comparison between simulated and measured results is obtained when looking at the spectral dependence of  $j_{ph}$  and  $j_{SC}$ . The number of absorbed photons / generated electrons per m<sup>2</sup> aperture and nm wavelength for the measured planar sample (blue dots), the measured textured sample (red dots) and the simulated average (brown line) are given in Figure 5.

We find that per trend the simulation overestimates the generation for lower wavelengths and underestimates it for higher wavelengths. Literature values indicate an internal quantum efficiency of approx.. 90% for microcrystalline silicon solar cells at 600 nm wavelength [10]. Assuming similar collection efficiencies also at other wavelengths, these results indicate that the simulated average is a good description for short wavelengths but underestimates the absorption provided by the texture for higher wavelengths.



**Figure 5:** Measured spectrally resolved generated photocurrent density for the untextured sample (blue) and a textured sample (red). Also shown is the simulated spectrally resolved absorbed photocurrent density for the average of the ten structures (brown line).

Looking at Figure 4, we find that apart from the average also structure number 6 yields a simulated current that is very close to the measured one. One possibility could be to use a single, representative periodic structure feature to describe the optical characteristics of the random structure. However, when comparing the spectral dependence of structure number 6 to the measured one, we find that the average gives a much better resemblance than the single texture (not shown in Figure 5). This is a further argument to justify the use of the average for the simulation of the optical characteristics.

### 4 SUMMARY & CONCLUSIONS

We have introduced and investigated a method for the 3D optical simulation of scattering surfaces for thin film crystalline silicon solar cell. The method is based on an investigation of a scattering structure and the detection of the single structure features. Subsequently the detected geometrical properties of the single features are used to construct and implement the solar cell into the rigorous coupled wave analysis (RCWA). RCWA is then used to calculate the optical near- and farfield characteristics like reflection, transmission and absorption.

As an exemplary structure we have investigated a surface of sputtered and etched ZnO (Figure 1). On this surface we have identified ten single structure features and have implemented them into RCWA (Figure 2).

The absorption of a microcrystalline silicon solar cell deposited on the single structure features was calculated. In a first, simple assumption the average of this absorption was used to compare the simulated absorbed photocurrent based on absorption results to the simulated short circuit current density based in quantum efficiency measurements on large areas. We found good agreement between the calculated absorbed photocurrent and the calculated short circuit current.

In a more detailed investigation of the spectral dependence we found that the simulation probably underestimates the absorption for higher wavelengths. For a more detailed analysis further investigations and comparison to more and different samples are required.

Assuming that the approach of averaging the result is valid, the introduced method can be used to identify defined periodic structures that can lead to a higher efficiency than the random structure. In the investigated example we found one structure that could increase the absorbed current by up to  $3 \text{ mA/cm}^2$ .

A quick comparison of the geometrical characteristics showed additionally, that structure features with small diameters are preferable. The best result was achieved for a feature with a diameter of D = 800 nm.

# 5 ACKNOWLEDGMENTS

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