

Electro – optical simulation of diffraction in solar cells

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Abstract: A simulation method is presented and evaluated for simulating two- and three dimensional wave optical effects in crystalline silicon solar cells. Due to a thickness in the 100 μm range, optical properties of these solar cells typically are simulated, primarily through the use of ray-tracing. Recently, diffractive elements such as gratings or photonic crystals have been investigated for their application in crystalline silicon solar cells, making it necessary to consider two- and three dimensional wave optical effects. The presented approach couples a rigorous wave optical simulation to a semiconductor device simulation. In a first step, characteristic parameters, simulated for a reference setup using the electro-optical method and the standard procedure are compared. Occurring differences provide a measure to quantify the errors of the electro-optical method. These errors are below 0.4% relative. In a second step the electro-optical method is used to simulate a crystalline silicon solar cell with a back side diffractive grating. It is found that the grating enhances to short circuit current density j_{SC} of the solar cell by more than 1 mA/cm^2 .

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1. Introduction

Light trapping based on optical nanostructures is one key feature of solar cell research [1–5] today. For the simulation of optical effects induced by nanostructures, rigorous wave optical methods are required. For the simulation of solar cells, optical as well as electrical effects need to be considered. Simulation methods for crystalline silicon solar cells that are capable of considering two- and three dimensional effects of wave optics are not state of the art. Typically, optical properties of crystalline silicon solar cells are simulated using a combination of ray tracing and transfer matrix method [6].

In this paper we present a coupled simulation method to consider wave optical effects in crystalline silicon solar cells. For this purpose the optical simulation within the semiconductor device simulation tool Sentaurus Device (SD) is substituted by a wave optical simulation using the rigorous coupled wave analysis (RCWA). We use thin crystalline silicon solar cells for several reasons. Reaching thicknesses well below 50 μm in the lab, conventional light trapping techniques are not sufficient to provide an effective absorption of the red part of the solar spectrum. Diffractive structures are one way to achieve sufficient path lengths. Furthermore, crystalline silicon solar cells are very well understood and therefore constitute a reasonable choice as a reference system. The presented method should, without much effort, also be transferrable to other solar cell systems.

In the first part of the paper we investigate and evaluate this substitution based on the example of a simple reference system. The reference system comprises no nanostructures and can therefore be simulated correctly with SD as well as with the coupled method. By comparing results obtained with both methods, we specify confidence intervals and operating conditions for the coupled method. In the second part of the paper we use the coupled method to simulate a crystalline silicon solar cell with a diffractive grating and compare the results to those of a simulated solar cell without grating. We show that diffractive effects influence the simulated electrical properties and that these effects can be simulated reliably using the presented method.

The idea to use diffractive gratings in solar cells was first formulated by Ping Sheng et al. [7]. Investigations of gratings for crystalline silicon solar cells have been performed by Heine & Morf [8]. Recently, interest in this topic has renewed for silicon thin film solar cells [9] as well as for organic solar cells [10]. Apart from gratings, diffractive photonic crystals were proposed in [11]. Works related to the method introduced in this paper were presented by Voisin [12] and Janz [13].

2. Simulation methods

In this section we give a short overview of the simulation tools used. These tools are the rigorous coupled wave analysis (RCWA) and the TCAD environment Sentaurus Device (SD).

2.1 Rigorous coupled wave analysis – RCWA

The coupled method requires information about the optical near- as well as the far field. Near field information is needed to calculate the local absorption in the solar cell, and far field information is needed to calculate reflection, transmission and absorption spectra.

Several methods exist for a rigorous wave optical simulation of the electromagnetic field inside a certain structure. Examples include, among others, Fourier modal methods (FMM), of which RCWA is an example, finite difference time domain (FDTD), and finite elements (FE). All of these methods can be used for the task discussed here. RCWA was developed for the simulation of diffractive gratings, for which it is especially efficient. A diffractive grating serves as an exemplary system in the second part of the paper. An early version of the RCWA method was formulated for the simulation of optical properties of sinusoidal gratings by Burcardt [14]. The method was further developed by Kogelnik [15]. A detailed description of the method used in this paper and how to implement it is given by Moharam [16]. The code used for the simulations in this paper was implemented by Lalanne [17] in a MATLAB environment.

2.2 *Sentaurus Device* - SD

For the simulation of electrical solar cell properties, the semiconductor device simulation program Sentaurus TCAD, released by the company Synopsys, was used. One tool of this program is Sentaurus Device (SD), which was mainly used for the simulations. SD features a modular routine to simulate solar cells [18]. Different parts of the simulation are performed in different modules of the tool. The modules are executed sequentially and produce input files for the subsequent modules. This procedure permits to alter the program during simulation by changing the input files. In the method presented here, the output file of the module for the simulation of optical properties is exchanged with another file that was simulated using RCWA. Important here is that the structure of the externally generated input file matches the internal requirements of SD and incorporates information such as the mesh in use or the material parameters [19]. The input file contains information about how much light of a certain wavelength is absorbed at a certain depth of the solar cell. This input file will be referred to in the text as the “absorption profile” (see Fig. 3).

A further remark has to be made about the absorption profile. Initially, the absorption within the solar cell is a 3D function of space. To reduce this function towards a 1D absorption distribution along the depth (z-axis) of the solar cell, a projection has to be chosen. The projection used in this paper is that the z-coordinate of a certain point within the solar cell is given by the minimum distance to the solar cell front surface. For the presented setup, this projection is straightforward. For textured front surfaces, however, the projection marks a critical issue.

3. Exemplary systems

In this section we describe the solar cells investigated in this paper. In the first part, the effects of substituting the optical simulation method of SD by an RCWA simulation are evaluated. For this purpose we chose a simple solar cell geometry that exhibits no diffractive effects and can be simulated correctly by SD as well as the coupled method. This simple setup is shown in Fig. 1a. The investigated solar cell has a flat front surface and a thickness of $d = 40\mu\text{m}$. It is equipped with an antireflection (AR) coating and a perfect back side reflector. The AR coating consists of a 67.8 nm thick SiN layer, the material parameters of which were measured in-house. The reflector is separated from the silicon by a 1 μm SiO₂ buffer layer.

In the second part of the paper we investigate the effects induced on a crystalline silicon solar cell by a back side grating. For this purpose, electrical and optical properties of the solar cell shown in Fig. 1a are compared to those of a solar cell with back side grating (Fig. 1b). Between SiO₂ and Si, a binary grating is positioned. The parameters of the grating are: grating period $A = 370\text{ nm}$ and groove depth of $d = 120\text{ nm}$. These parameters have been chosen according to earlier studies [20].

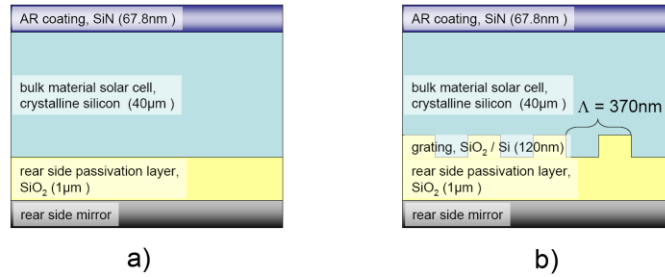


Fig. 1. Sketch of the solar cell geometries investigated in this paper. Figure 1a shows the solar cell geometry used for evaluating the substitution of optical simulation tools and used as a reference for the investigation of grating effects. Figure 1b shows the solar cell geometry used to simulate the effects of a diffractive grating in a crystalline silicon solar cell.

A further remark has to be made about the properties of the back side mirror. In different simulation methods, a perfect back side mirror is realized in different ways. In SD the ray tracing routine allows modeling a perfect back side mirror by setting the reflectance at the rear side to 1. This is not possible for methods based on Maxwell's equations. Here either very good dielectric mirrors need to be implemented or materials with very high absorption coefficients need to be assumed. In this paper, a perfect mirror was implemented by using a material with $n = k = 100$.

Not shown in Fig. 1 are several features required for an electrical solar cell simulation. These features are for example the presence of a P/N junction in the bulk material and electrical contacts at front and rear surface. For an electrical simulation also several additional parameters need to be considered. As most of them are not relevant for the presented investigation, they are not mentioned here. One parameter that is relevant is the surface recombination velocity S_0 . Here equal values were used for a solar cell with and without grating. Assumed are standard values from Sentaurus Device for crystalline silicon solar cells. These values are $S_0 = 10^3$ cm/s at the front surface and $S_0 \approx 2 \cdot 10^6$ cm/s at the rear surface.

4. Evaluation of coupled method

In this section we investigate in how far a substitution of the optical simulation in SD by RCWA simulations influences the characteristic parameters calculated for the simple cell geometry shown in Fig. 1a. Three different parameters are investigated and compared for this purpose. The first parameter is the spectral absorption from which the absorbed photocurrent density j_{ph} is calculated. The second parameter is the absorption profile, the input for the electrical simulation. Finally, as a third parameter, the current voltage characteristics are calculated.

4.1 Comparison of the spectral absorption

In a first set of simulations, the spectrally resolved total absorption of the system was simulated. The quantity used to compare the different methods is the photocurrent density j_{ph} which is calculated by

$$j_{ph} = -e_0 \int d\lambda \text{abs}(\lambda) \Phi_{AM1.5g}(\lambda) \quad (1)$$

In Eq. (1) e_0 is the elementary charge, $\text{abs}(\lambda)$ is the absorption of the entire system per wavelength and $\Phi_{AM1.5g}$ is the photon flux in the AM1.5g solar spectrum per wavelength. The used solar spectrum was taken from SD; small differences occur if other spectra are used. The photocurrent density contains all absorbed photons; losses are not considered. The results of these simulations are shown in Fig. 2. Figure 2a shows the results of the reference simulation with SD. This result has to be retrieved using RCWA in order to arrive at a reliable substitution. Figure 2b shows the result of a single RCWA simulation of the absorption for the same solar cell geometry. The RCWA method performs a completely coherent simulation of

the given geometry. For this reason, strong interference effects are noticeable. These effects manifest as strong oscillations for wavelengths above $\lambda > 800 \text{ nm}$ and also for shorter wavelengths, if the silicon thickness is a multiple of the considered light wavelength. The calculated photocurrent density for this oscillating spectrum is approx. 0.4 mA/cm^2 above the value calculated with SD.

To approach the result obtained with SD, interference effects need to be eliminated in all layers the thickness of which exceed the coherence length of sunlight in the considered solar spectrum (approx. $1 \mu\text{m}$). In the investigated setup, this is the case for the silicon bulk layer ($d = 40 \mu\text{m}$). To eliminate interference effects, we have performed several steps. The first step was to avoid wavelengths for which resonant effects occur. With this procedure, all elopers below $\lambda = 800 \text{ nm}$ could be eliminated (see Fig. 2b). The second step was to perform a variation of either the wavelength or the silicon thickness and to average over the simulations. With both variations similar results are obtained. A variation of the silicon thickness of $\pm 0.4 \mu\text{m}$ in nine steps turned out to be an efficient procedure. The result of these strategies is shown in Fig. 2c. Interference effects are efficiently suppressed and the deviation in photon current density is reduced to approx. $\Delta j_{ph} = 0.14 \text{ mA/cm}^2$ corresponding to a relative difference of approx. 0.4%.

A further remark needs to be made about the back side reflector. A difference between SD and RCWA is that in the RCWA simulation, the back side mirror absorbs some radiation, whereas in SD it doesn't. The higher photo current density obtained with the RCWA simulation can partly be explained with this additional absorption. A simple estimation resulted in an absorbed photo current density in the back side reflector of approx. 0.2 mA/cm^2 .

With the presented corrections, the difference between the photocurrent densities calculated with SD and RCWA is below $\Delta j_{ph} = 0.1 \text{ mA/cm}^2$ for the investigated solar cell geometry. Effects which result in current density differences smaller than this value cannot be investigated reliably with the electro-optical method. Furthermore, we will use the obtained value as an error for short circuit current densities for comparable geometries to indicate the confidence interval provided by the method.

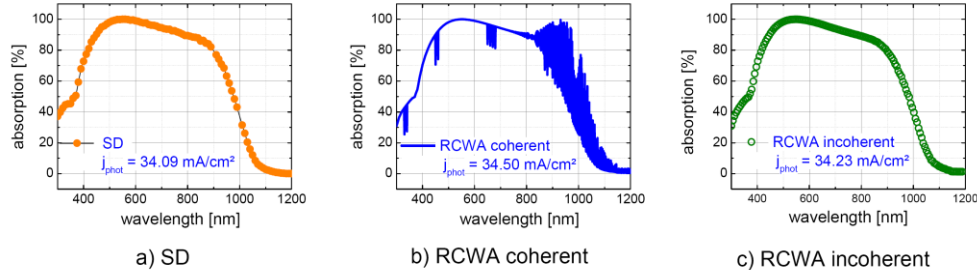


Fig. 2. Absorption spectra simulated using SD and RCWA. Also given are the photocurrent densities corresponding to each spectrum. Figure 2a shows the reference spectrum calculated with SD. Figure 2b shows the spectrum for the same system calculated with RCWA by a single simulation. Strong interference effects are noticeable. In Fig. 2c interference effects have been eliminated by averaging over several calculations for which the silicon thickness has been varied.

4.2 Comparison of the absorption profile

The absorption spectrum is not the only source of differences between the coupled method and SD. The current generation inside a solar cell does not only depend on the amount of light absorbed but also on the position of the absorption within the solar cell. In a second set of simulations, the spectral and spatial distribution of the absorption for different simulation procedures was calculated. The results of these simulations are shown in Fig. 3.

The simulations presented are confined to a spectral range between $800 \text{ nm} < \lambda < 1200 \text{ nm}$. The restriction has been performed because a simulation of the entire spectrum requires a lot of time and computer resources. For this reason the simulation was limited to the spectral

range in which the effects of nanostructures investigated later with this method are expected. To ensure that only effects due to differences in the spatial absorption distribution are considered, the spectral absorption distribution was equal in all cases.

The absorption profile calculated with SD is shown in Fig. 3a. This profile serves as reference for the comparison with the coupled method. Using this file to simulate the short circuit current density, a value of $j_{SC} = 11.40 \text{ mA/cm}^2$ is obtained (note that only a part of the solar spectrum is considered, thus the difference to the photocurrent density).

To calculate the absorption profile from RCWA simulations, the theorem of Poynting [21] was used.

$$Abs(\vec{r}, \omega) = \frac{1}{2} \omega \epsilon_0 \epsilon''(\omega) |E(\vec{r}, \omega)|^2 \quad (2)$$

In Eq. (2) $Abs(\vec{r}, \omega)$ is the spectrally and spatially dependent absorption, $\epsilon''(\omega)$ is the imaginary part of the dielectric function and $E(\vec{r}, \omega)$ is the spectrally and spatially dependent electric field. The latter is a result of the RCWA simulation.

Figure 3b shows the absorption profile for the chosen solar cell geometry calculated with a single RCWA simulation. As in the absorption spectrum (Fig. 2b), strong interference effects are noticeable. Performing electrical simulations, the profile shown in this figure generates a short circuit current density of $j_{SC} = 11.45 \text{ mA/cm}^2$. The difference to the result obtained with SD is already small, even for strong differences in the local absorption distribution. Interference effects are again reduced by averaging over several simulations of the electric field for which the thickness of the bulk silicon is varied. The result for a variation over $\pm 0.4 \mu\text{m}$ in nine steps is shown in Fig. 3c. Noticeable differences to the result obtained with SD remain especially close to the solar cell surface. After calculating the short circuit current density generated by this absorption profile, however, no significant difference to the result obtained with SD remain ($j_{SC} = 11.40 \text{ mA/cm}^2$).

A further reduction of interference effects is achieved by applying an exponential fit to the spatial absorption function close to the solar cell front surface. Interference effects can be eliminated completely in that way. This procedure has to be handled with care, however, as assumptions about the absorption distribution function must be made a priori. Compared to the differences in the spectral absorption, the differences caused by deviations in the spatial absorption distribution are comparably small and may be neglected. Expressed differently, for the generated current density, the amount of absorbed light is more important than the spatial distribution of the absorption, at least for the investigated geometry.

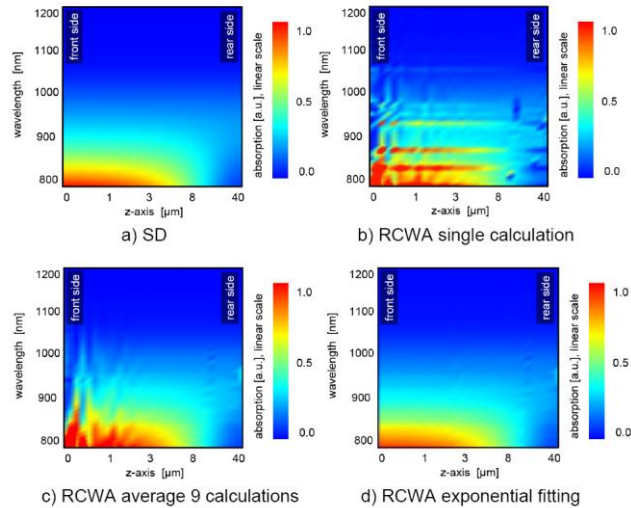


Fig. 3. Absorption profiles calculated with SD and RCWA. Figure 3a shows the absorption profile calculated with SD. The generated short circuit current density is $j_{SC} = 11.40 \text{ mA/cm}^2$. Figure 3b shows the result obtained with a single RCWA calculation. Strong interference effects are noticeable. The current density here is $j_{SC} = 11.45 \text{ mA/cm}^2$. Figure 3c shows the average over nine RCWA simulations with a small variation of the silicon thickness. Coherent effects are reduced, $j_{SC} = 11.40 \text{ mA/cm}^2$. Figure 3d shows the result of an additional exponential fit; $j_{SC} = 11.40 \text{ mA/cm}^2$. Note that the z-axes are scaled non-linearly. The absorption is given in relation to 100% incident light for each wavelength.

4.3 Comparison of the electrical characteristics

In a last step, we have used the simulated optical properties discussed in the preceding paragraphs to perform electrical simulation of a crystalline silicon solar cell. The electrical solar cell properties have once been calculated using the standard procedure with SD as a reference. For this simulation, the optical characteristics shown in Fig. 2a and Fig. 3a were used. As diffractive effects are expected mainly in the spectral range above $\lambda = 800 \text{ nm}$, for smaller wavelength the optical properties simulated with the standard procedure have been used. Additionally, the electrical solar cell characteristics have been calculated using the coupled method. Here the optical characteristics shown in Fig. 2c and Fig. 3c were used. The result of the electrical simulations is shown in Fig. 4.

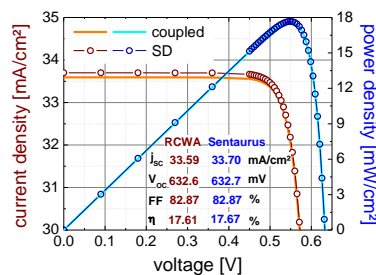


Fig. 4. Electrical characteristics of a solar cell simulated using the coupled method (lines) and the standard procedure with SD (circles). Shown are the current voltage relation (orange / brown) and the power voltage relation (cyan / blue). Small deviations in the characteristics occur that are caused by differences in the total absorption. The significant deviations occur for j_{sc} ; $\Delta j_{sc} = 0.11 \text{ mA/cm}^2$ and for efficiency $\Delta \eta = 0.06\%$ absolute.

Using the coupled method instead of the standard procedure, small deviations in the obtained short circuit current density and efficiency occur. These deviations are caused by

differences in the simulated total amount of absorbed light. Differences in the spatial absorption distribution have only marginal effects. The most significant difference for the coupled method is the one in short circuit current density. In the investigated example, this difference is $\Delta j_{SC} = 0.11 \text{ mA/cm}^2$ corresponding to approx. 0.35% relative. The same relative difference is found for the efficiency, corresponding to $\Delta \eta = 0.6\%$ in absolute terms.

At the current stage of development, the presented procedure provides a good compromise between expense in time and computer capacity and the resulting differences between the coupled method and SD. A further reduction of these differences is possible by increasing the number of calculations used for the averaging process and an accompanying further reduction of interference effects.

Compared to SD, the deviations in the results obtained with the coupled method can be interpreted as confidence intervals. We will express this in the following text by using the deviations as error values to indicate the magnitude of uncertainty provided by the coupled method. This procedure is restricted to solar cell systems similar to the one investigated up until now.

5. Simulation of a solar cell with diffractive back side grating

In this section we investigate a system that cannot be simulated by standard ray tracing procedures. The investigated system is a crystalline silicon solar cell with a diffractive back side grating (Fig. 1b). The grating changes the distribution of radiation inside the solar cell resulting in an increased absorption. This diffraction effect can only be simulated with two- and three dimensional wave optical methods. We compare optical and electrical characteristics of a solar cell with and without grating (Fig. 1a) using the presented coupled method.

5.1 Absorption spectrum and absorption profile

We start with a comparison between the simulated absorption spectra of a solar cell with and without grating (Fig. 5a) using RCWA. Shown are the two absorption spectra (blue and cyan line) as well as the difference between these spectra (brown circles) in absolute %. The grating causes a considerable increase in absorption in the spectral range around $\lambda = 990 \text{ nm}$. Calculating the photocurrent densities using Eq. (1), the increased absorption results in an increase in photocurrent density of $\Delta j_{ph} = 1.2 (\pm 0.1) \text{ mA/cm}^2$.

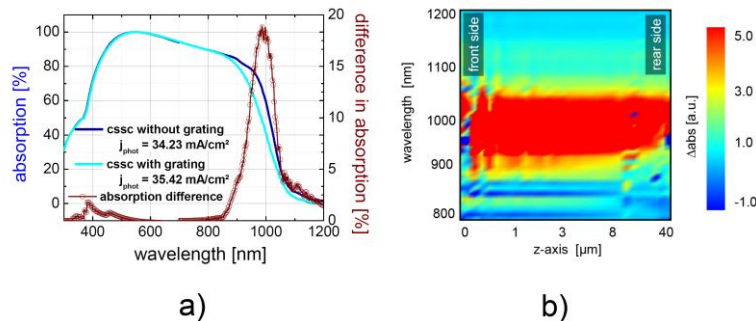


Fig. 5. Figure 5a shows the absorption spectra for a crystalline silicon solar cell with and without grating (blue and cyan line) as well as the difference between these spectra (brown circles). The grating causes an increase in absorption of up to 20% around $\lambda = 990 \text{ nm}$ resulting in an increase in photocurrent density of $\Delta j_{ph} = 1.2 (\pm 0.1) \text{ mA/cm}^2$. Figure 5b shows the difference of the corresponding absorption profiles (cf. Figure 3).

Figure 5b shows the spatial distribution of the additional absorption induced by the grating. The distribution was calculated by subtracting the absorption profile for a crystalline silicon solar cell without grating (Fig. 3c) from the absorption profile of a solar cell with grating. The figure shows that the absorption increase in the wavelength range around $\lambda = 990$

nm is distributed evenly throughout the cell. Oscillations are caused by interference effects that were not eliminated completely by averaging processes.

5.2 Electrical characteristic

Finally, the coupled method has been used to calculate the electrical characteristics of a crystalline silicon solar cell with and without grating. The absorption profiles used for this simulation are the ones also used to calculate Fig. 5b. The result of the electrical simulation is shown in Fig. 6.

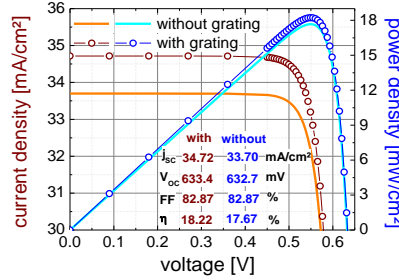


Fig. 6. Electrical characteristics for a crystalline silicon solar cell with (lines) and without (circles) grating. Given are the current voltage relation (brown / orange) and the power voltage relation (blue / cyan). The grating induces an increase in short circuit current density of $\Delta j_{sc} = 1.02 (\pm 0.11) \text{ mA/cm}^2$ and an increase inefficiency of $\Delta \eta = 0.55 (\pm 0.06) \%$ absolute.

The increased absorption induced by the grating causes an increase in short circuit current density of $\Delta j_{sc} = 1.02 (\pm 0.11) \text{ mA/cm}^2$. The increase in short circuit current density therefore images the increase in photocurrent density. The increased short circuit current density is passed directly to an increase in efficiency of the same relative magnitude and with an absolute value of $\Delta \eta = 0.55 (\pm 0.06) \%$. The error values used here are the ones obtained from the comparisons in section 4.

Two conclusions can be drawn from the results of this simulation. The first conclusion is that the presented method can be used to investigate theoretically the effects of diffractive structures in solar cells, provided the effects exceed the level of uncertainty. The second conclusion is that a considerable improvement of a crystalline silicon solar cell can be achieved by the introduction of a diffractive grating.

6. Summary and outlook

In summary, we introduced and discussed a method for the simulation of two – and three dimensional wave optical effects in solar cells. The presented method is based on coupling the rigorous wave optical simulation method RCWA to the semiconductor device simulation tool SD. RCWA is used to simulate the optical properties of a solar cell system. The results of this simulation are used as input for an electrical simulation with SD.

In the first part of the paper the coupled method was evaluated. For this purpose, a simple exemplary setup without diffractive elements was implemented. The setup consisted of a flat crystalline silicon solar cell with a thickness of $40\mu\text{m}$, an AR coating and a backside mirror. This setup can be simulated correctly using SD as well as the coupled method. A first comparison showed that interference effects cause considerable deviations for RCWA simulations when compared to standard procedure results. To reduce these differences we developed a method based on averaging over multiple simulations. With this procedure we achieved a difference in the absorbed photocurrent density of below $\Delta j_{ph} = 0.1 \text{ mA/cm}^2$ corresponding to less than 0.3% absolute.

In a second step, a simulation of the electrical solar cell parameters was performed using the coupled method and the standard procedure. Differences in the results obtained here mark uncertainties of the coupled method. The significant difference is the one for the short circuit current density j_{sc} . Here we obtained $\Delta j_{sc} = 0.11 \text{ mA/cm}^2$ corresponding to a relative value of

0.35%. The same relative difference is obtained for the efficiency; $d\eta = 0.06\%$ in absolute terms.

In the second part of the paper, we used the coupled method to investigate the effects of a diffractive grating on the electrical characteristics of a crystalline silicon solar cell. This setup cannot be calculated with the standard procedure. In a first step, the optical properties of a solar cell with and without grating were simulated using RCWA. We found that the implemented grating induced an increase in absorption corresponding to an increase in j_{ph} of $\Delta j_{ph} = 1.2 (\pm 0.1) \text{ mA/cm}^2$. Subsequently, we performed electrical simulations using the coupled method. Here we found that the grating increases the short circuit current density by $\Delta j_{sc} = 1 (\pm 0.1) \text{ mA/cm}^2$ and the efficiency by $\Delta\eta = 0.55 (\pm 0.06)\%$ absolute. The relative increase in both cases is 3%.

With the presented method, a tool exists that can be used for the simulation and optimization of diffractive gratings for solar cells. A parameter variation with the aim to maximize the increase in efficiency will be a next step. Furthermore, the method shall be extended towards other structures like photonic crystals. The consideration of front surface textures is a challenge, because large structures with typical sizes in the μm regime cannot easily be considered with the presented method. To solve this problem, we are currently working on a method based on an improved ray tracing approach.

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