Light Trapping in High-Efficiency Crystalline Silicon Solar Cells

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1 Introduction

1.1 Motivation: From sunlight to electric energy

Climate change due to anthropogenic greenhouse gas emissions, decreasing resources of fossil energy and risks related to power generation in nuclear power plants challenge the previously dominating ways of energy conversion. The current human power demand sums up to approximately 0.02 PW [1]. The solar radiation incident on the earth equates to a power input of 174 PW, which suggests that a conversion of the solar radiation by photovoltaics (PV) can significantly contribute to cover the energy demand. According to [2], the direct conversion of solar radiation by PV has a very large sustainable potential exceeding the worldwide energy demand by far.

To exploit this potential, photovoltaic energy conversion has to be efficient and reliable and consequential economically competitive. Since the first silicon based solar cells in the mid of the 20th century, continuous research has driven efficiencies up and cost down. The fundamental limit of a semiconductor-based solar cell with a single band gap material has been assessed by Shockley and Queisser [3] and reassessed for crystalline silicon solar cells by Richter et al. [4] yielding a maximum efficiency of 29.4%. Up to date, the most efficient silicon solar cell reaches 26.7% [5] and typical industrial silicon solar cells in mass production feature efficiencies between 18 and 23% [6]. Any further efficiency increase can reduce cost, material and energy consumption in the production of cells and modules, demand for land etc. – important steps to a system based on renewable energy sources. Over the last 40 years, the inflation adjusted cost per watt of a PV module already decreased by 22.5% for every doubling of the cumulative production, leading to an annual installation of approx. 75 GWp and 0.37 $/Wp in 2016 [6]. In order to follow this path of reducing cost and increasing installations, scientific innovations are required. Increasing the efficiency of solar cells still is an important lever, because many costs in a complete system (especially all area-related costs) can be reduced when the cell efficiency is increased.

To enable further efficiency enhancements, improving the optical properties of silicon solar cells is one possibility and will be the focus of this work. According to [6], the thickness of industrial silicon solar cells will further reduce to below 150 µm in the next 10 years. In order to avoid increasing absorption losses in thinner solar cells and to optimize optical and electrical properties simultaneously, this work develops and investigates novel surface structures that allow for long light path lengths even in thin crystalline silicon solar cells and thus for efficient light trapping while also reaching very good electrical properties and overall high efficiencies.
1.2 Light trapping in silicon solar cells

Crystalline silicon as semiconductor with an indirect band gap only weakly absorbs light. For each photon (with a wavelength higher than 380 nm) to be absorbed within silicon, an additional phonon is required. Thus silicon solar cells require an absorber that is much thicker than in the case of direct semiconductors. Especially in the wavelength range close to the bandgap (1108 nm), the absorption coefficient of crystalline silicon gets very weak, leading to penetration depths of several mm. Solar cells with an absorber thickness of several mm would suffer from serious electrical losses due to recombination. Thus light path lengths have to be increased in the silicon without increasing the absorber thickness. This can be reached by structuring the surfaces of a solar cell. Well established methods for structuring the front of silicon solar cells comprise wet chemical etching of pyramids (mono-crystalline silicon) or of round-shaped isotextures (multi-crystalline silicon). In scientific literature, also diffractive gratings at the rear have been proposed already more than 20 years ago [7]. However, the works on diffractive gratings so far focused mainly on simulations, optical properties and proof-of-concepts and not yet on the integration of diffractive structures into high-efficiency silicon solar cells, where also the resulting electrical properties have to be considered. This is the goal of this work.

To improve light trapping, the combination of the front and the rear of the solar cell has to be optimized simultaneously. Very good antireflective properties have to be combined with light path length enhancing properties. Especially, when front and rear textures operate in different optical regimes, there are no well-established simulation tools available and thus the simulation formalism Optical Properties of Textured Optical Sheets (OPTOS) has been developed within this work. Various combinations of front and rear structures have been simulated and also realized experimentally.

To improve not only light trapping but the overall efficiency of a solar cell, all electrical properties, especially surface passivation and contact formation have to be considered while optimizing the optical properties. One possibility to combine both, very good light trapping and very good electrical properties, is a concept introduced within this work: solar cells that are electrically planar, but optically structured (EPOS). In EPOS solar cells, a very good electrical passivation can be ensured by a planar dielectric passivation layer and very good light trapping can be realized by adding an additional light-redirecting structure that does not alter the electrical surface passivation.

To improve solar cells beyond the limits for silicon single-junction solar cells, tandem devices based on a silicon bottom solar cell are a promising approach. With tandem devices, the Shockley-Queisser limit can be exceeded, but current tandem devices – III/V on silicon as well as perovskite on silicon – suffer from low current densities in the silicon bottom solar cell. Thus, the light trapping concepts developed in this thesis are especially important for such tandem devices.
1.3 Objectives of the thesis

To realize an optimized light trapping in high-efficiency crystalline silicon solar cells, this work pursues the following main objectives:

- Developing methods to efficiently simulate various combinations of light trapping structures at the front and rear of silicon solar cells. These structures may operate in different optical regimes. The simulations have to be experimentally verified. Based on these simulations, this thesis wants to give an overview over various light trapping concepts and identify promising front and rear structure combinations.

- Investigation of alternative antireflection structures: multilayer planar coatings and black silicon. Both concepts are investigated especially with respect to possible combinations with additional light trapping structures at the rear. Optimizations of antireflection structures are also evaluated in the context of modules, where further layers like encapsulation materials or a front glass have to be considered.

- Integrating diffractive gratings into high-efficiency crystalline silicon solar cells. Therefore, two approaches are followed: hexagonal sphere gratings and binary crossed gratings. For both concepts, not only improved light trapping is targeted but an improved overall efficiency compared to reference solar cells without diffractive rear side gratings.

- Benchmarking all novel concepts against state-of-the-art techniques and simple approaches. Therefore also simple diffuse rear reflectors like white paint are investigated and compared.

- Showing the potential of the developed concepts for the field of silicon based tandem solar cells.

Overall, this thesis tries to combine improvements of the optical properties of silicon solar cells with very good electrical properties. This requires, besides the fundamental optical investigations, also work related to the actual processing of solar cells. All changes that are made to a high-efficiency silicon solar cell to improve the optics have to be done in a way that electrical properties are – at least – not deteriorated. Therefore, this thesis wants to demonstrate that also complex optical structures can be integrated into high-efficiency crystalline silicon solar cells beneficially.
1.4 Outline of the thesis

In the following Chapter 2, I am going to provide the theoretical background for this thesis: basics for the understanding of silicon solar cells with a focus on optics. An overview over light trapping concepts and light trapping limits is given and the concept of electrically planar but optically structured solar cells is presented.

Chapter 3 starts with a presentation of the used standard methods for the simulation of the optical properties of silicon solar cells. Then, it focusses on the development of the simulation formalism OPTOS, from 2D structures and two interfaces to 3D structures and several interfaces. Detailed validations as well as examples for the application of OPTOS are shown.

Alternative antireflection systems are investigated in Chapter 4. Multilayer planar antireflection coatings and black silicon as two possible alternatives to standard front side textures are examined, also with respect to the possible combination with additional rear structures.

Chapter 5 is dedicated to the experimental realization of light trapping structures. First, simple diffuse rear reflectors as benchmark are presented, second binary gratings and, third, sphere gratings for the rear are integrated into crystalline silicon solar cells. For all light trapping structures, I conducted process development, optical and electrical characterization and processing of full solar cells.

A detailed comparison of different light trapping structures and structure combinations is given in Chapter 6. Simulations as well as experimental results are included in this chapter. Finally, it also gives an outlook towards silicon based tandem solar cells and the possible benefits of the developed light trapping structures to tandem devices.

Chapter 7 summarizes the thesis in English and Chapter 8 in German.
In this chapter, I will outline the theoretical background needed for this work. The fundamental working principle of a silicon solar cell is presented briefly. In the subsequent sections I will discuss the theoretical background for realizing silicon solar cells with optimized light trapping. This includes light trapping limits and light trapping concepts, but also the electrical passivation and contact formation. In addition to the mere theoretical background, this chapter also contains comparative studies of light trapping limits and finally leads to the introduction of a novel concept that will be one key aspect of the following work: a solar cell that is electrically planar but optically structured.

2.1 The origin of the solar cell’s IV characteristics

A photovoltaic solar cell has to convert incident solar radiation (or photons) into electrical power. Such a conversion in a semiconductor is based on the photo-electrical effect discovered by Edmont Becquerel in 1839 [8]. Using a simplified picture, this conversion can be separated into several steps: first absorption of the incident photons, which creates electron hole pairs within the silicon, second separation of these free charge carriers and third conduction of the separated charge carriers to an external circuit. At first one has to consider the input, which is the solar spectrum. The solar spectrum changes while passing the earth’s atmosphere. Within this work, always the air mass 1.5g (AM 1.5g) standard spectrum as defined by the International Electrotechnical Commission IEC [9] is used. This is related to the global radiation (direct and diffuse) after passing the atmosphere 1.5 times, which is related to a direction of propagation with an angle of approx. 48° to the normal. The real part \( n \) and the imaginary part \( k \) of the refractive index of crystalline silicon determine what happens to the light incident on a crystalline silicon solar cell. The imaginary part of the refractive index is related to the absorption coefficient \( \alpha \) by \( \alpha = \frac{4\pi k}{\lambda} \). The absorbance \( A \) of light with a specific wavelength after a path length of \( x \) inside the silicon can be calculated by Lambert-Beer’s law \( A(x) = 1 - \exp(-\alpha x) \). The penetration depth \( \delta = \frac{1}{\alpha} \) denotes the path length after which the intensity is decreased by a factor 1/e. Figure 1 shows \( n, k, \alpha \) and \( \delta \).
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Figure 1: Refractive index $n$ and $k$, absorption coefficient $\alpha$ and penetration depth $\delta$ for crystalline Silicon at 300 K. Data from Green [10].

These optical quantities explain the absorption only phenomenologically and to understand the process of absorption one has to consider the band diagram of Si, which has an indirect bandgap at 1.12 eV. The characteristic of the absorption coefficient depicted in Figure 1 can be explained by the possible transitions from valence to conduction band including phonon assisted processes [11]. After the absorption process, the generated electrons and holes have to be separated. In a simplified model, a pn-junction that creates an electric field in the depletion region leads to this charge carrier separation [12]. Also the different mobilities of minority and majority charge carriers in different regions of the solar cell can be understood as reason for a charge carrier separation. The exact mechanisms how this separation can be realized, understood and best described are still under discussion [13]. For the following work this is not of major importance and we can follow the simplified theory of a mere pn-junction. The simplest description of a pn-junction is given by the one-diode equation. Based on this, a solar cell under illumination delivers the following current density $J$:

$$J(V) = J_0 \left( \exp \left( \frac{qV}{kT} \right) - 1 \right) - J_L,$$

where $J_0$ is the dark saturation current density, $q$ the elementary charge, $V$ the voltage, $k$ Boltzmann’s constant, $T$ the temperature and $J_L$ the current density induced by light absorption and subsequent charge carrier separation. The most important quantities used to describe a solar cell, $J_{SC}$, $V_{OC}$ and $FF$ can be deduced from this formula. The open circuit voltage $V_{OC}$ describes the voltage, where the current density $J(V)$ of the solar cell is zero:

$$V_{OC} = \frac{kT}{q} \ln \left( \frac{J_L}{J_0} + 1 \right).$$

The short circuit current density describes the current of a solar cell at $V = 0$ and in the notation used above we get $J_{SC} = -J_L$. An exemplary $JV$ curve is plotted in Figure 2 for an exemplary set of parameters. $J_{SC}$ and $V_{OC}$ are directly visible in such a plot. At both these points in the $JV$-curve,
2 Working principles of solar cells

however, no electrical power can be extracted from the solar cell. There is a so called maximum power point (MPP) where the electrical power density \( P = JV \) gets maximal. Knowing the current density \( J_{\text{MPP}} \) and voltage \( V_{\text{MPP}} \) at this point, the third fundamental parameter, the fill factor (FF), can be calculated:

\[
FF = \frac{V_{\text{MPP}}J_{\text{MPP}}}{V_{\text{OC}}J_{\text{OC}}}. \tag{3}
\]

Combining these three, the efficiency \( \eta \) of the conversion of light into electrical power is given by

\[
\eta = V_{\text{OC}}J_{\text{SC}}FF. \tag{4}
\]

Figure 2: Schematic JV-curve of a dark and illuminated solar cell.

The quantities described so far do not contain any spectrally resolved information. The external quantum efficiency (EQE) describes the efficiency of the conversion of one single photon with a specific wavelength into an electrical current. Considering AM 1.5g illumination, it is related to the short circuit current density by

\[
J_{\text{SC}} = -q \int_{0}^{\infty} \text{EQE}(\lambda)N_{\text{AM1.5g}}(\lambda) d\lambda, \tag{5}
\]

where \( N_{\text{AM1.5g}} \) is the spectral photon flux density. The external quantum efficiency is of major importance in this work. Many concepts in this work aim at improving the EQE in the near infrared. For every EQE one has to keep in mind that this quantity is only indirectly related to the efficiency of the solar cell, because voltage and fill factor are quantities quite independent from the EQE. In the literature also the internal quantum efficiency IQE is frequently used. It is defined by \( \text{IQE} = \frac{\text{EQE}}{1-R} \), where \( R \) depicts the reflectance. The IQE summarizes all other losses within the solar cell except of the reflectance. It is mostly used when electrical properties of the solar cell are optimized. For the
optical optimization it is less meaningful and therefore not used in this work. More complicated electrical models such as the two diode model introduce parallel and series resistance and different types of recombination. For the following work such approaches aiming at a more precise description of the electrical properties of solar cells, are not needed.

At each step described before, loss mechanisms occur. An incident photon may not create an electron hole pair or an electron hole pair may not be separated or conducted to the contacts. The fundamental loss mechanisms of a single junction solar cell are depicted in Figure 3. Photons with a wavelength larger than the bandgap cannot be absorbed and cause transmission losses. Photons with smaller wavelengths can be absorbed, but only the energy of the bandgap can be used. The excess energy leads to thermalization losses. The green area in Figure 3 gives the potentially usable energy. These fundamental loss mechanisms can also be quantified by a detailed balance analysis as done by Shockley and Queisser [3]. Reassessing the limiting efficiency of silicon solar cells with a similar approach including Auger recombination and further revised parameters for crystalline Si, Richter et. al calculated a maximum efficiency of 29.4% under one sun illumination [4].

![Figure 3: Thermalization and transmission losses in a silicon solar cell under illumination with AM 1.5g.](image)

Loss mechanisms further reducing the efficiency of real solar cells can be distinguished into optical and electrical losses. The electrical losses comprise recombination in the bulk and at surfaces, series resistance losses and parallel resistance losses. Optical losses comprise front surface reflection, weak absorption in the near infrared (NIR), also called absorption losses, and parasitic absorption. In a highly efficient solar cell, which aims at approaching the fundamental limits described above, all of these additional loss mechanisms have to be minimized. Thermalization and transmission losses cannot be minimized for a conventional single junction solar cell. The strategies of minimizing all other loss mechanisms that are important for this work are briefly introduced in the following sections 2.2 to 2.5 with a focus on the optical losses.
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2.2 Recombination losses and surface passivation

Recombination in general refers to the process reverse to generation: electrons and holes recombine without power being extracted from the solar cell. Every recombination process is characterized by a time constant, the recombination lifetime $\tau$, which gives the average time until an electron hole pair recombines:

$$\tau = \frac{\Delta n}{U},$$

where $\Delta n$ ($\Delta p$) is the excess carrier density of electrons (holes) with $\Delta n = \Delta p$ and $U$ is the recombination rate. There are different recombination mechanisms in crystalline silicon and the individual lifetimes $\tau_i$ add up to an effective lifetime:

$$\frac{1}{\tau_{\text{eff}}} = \sum \frac{1}{\tau_i}.$$  \hfill (7)

The most important recombination mechanisms are Auger recombination, radiative recombination and Shockley Read Hall (SRH) recombination. Auger recombination depends on the doping level but also occurs in intrinsic silicon [14], thus it cannot be fully eliminated and is considered for the fundamental limit of silicon solar cells [4]. Radiative recombination is of minor importance in crystalline silicon as it is an indirect semiconductor. Recombination facilitated by discrete energy levels within the band gap is called SRH recombination [15,16] and can occur in the bulk material (due to impurities, lattice defects etc.) or at the surface where so called interface traps create energy levels within the bandgap. There are two major strategies to reduce the recombination at surfaces. First, the reduction of the interface trap density $D_{it}$, and second, the field effect passivation. $D_{it}$ is typically reduced by dielectric surface passivation layers like SiO$_2$, SiN$_x$ or Al$_2$O$_3$. The field effect passivation reduces the minority charge carrier concentrations in the region close to the surface. This can be done by applying fixed charges at or near the surface (as for example in Al$_2$O$_3$, [17]) or by a high-low junction, which is used in case of a back surface field. Field effect passivation and $D_{it}$ reduction usually work in parallel.

For all concepts proposing advanced optical light trapping, the electrical surface passivation is of major importance, because when changing the surface in order to improve the optical properties one has to ensure, that an adapted passivation still effectively passivates the surfaces in order to reach high voltages.

2.3 Contact formation

In order to supply an external load, base and emitter have to be contacted separately to extract separated charge carriers out of the device. Usually metals like Ag or Al are used to contact the silicon base and emitter. A measure for the quality of the contact is the contact resistance that contributes to
the series resistance of the cell. As described in the section before, dielectric layers are used for passivation in highly efficient cells, which makes the contact formation more complicated. There are several methods to form local contact openings in an dielectric layer, like firing of metal pastes (e.g. [18]) or laser based processes (e.g. [19]). A well-known cell concept that features such local contacts is the Passivated Emitter and Rear Cell (PERC). Furthermore, there are concepts that combine passivation and contact formation. One of these concepts is the so called Tunnel Oxide Passivated Contact (TOPCon). It was introduced by Feldmann et al. [20,21] and features a very thin SiO$_2$ layer (1 to 2 nm) in combination with a poly-crystalline, doped Si-based layer. Very good electrical passivation and very low contact resistances leading to high efficiencies have been demonstrated (e.g. [22]). The contact in this case is a full area contact, in contrast to local contact openings for the PERC concept.

Especially for all concepts proposing advanced optical light trapping, the electrical contact formation is of major importance, because when changing the surface in order to improve the optical properties one has to change the contacts in order to prevent series resistance losses and to enable high fill factors.

### 2.4 Optics for silicon solar cells

The fundamental optical losses (transmission losses and thermalization losses) have already been presented in Figure 3. In this chapter, further optical losses are described: front surface reflection losses, absorption losses, and parasitic absorption. In the subsections 2.4.2 to 2.4.5, these losses are described in detail and possible ways to reduce them are presented. Beforehand, a brief section with important basics about optics in general is inserted here, trying not to repeat standard knowledge of textbooks.

#### 2.4.1 A brief introduction

Light as an electromagnetic wave can be described by Maxwell’s equations [23]. All further formulas and concepts presented can be deduced from these fundamental equations. Important for light trapping in silicon solar cells is the understanding of the interaction of light with a structured surface. There are different optical regimes that allow different approximations in order to simplify the description of the interaction of light with a structured surface. These regimes are separated by the different ratios of the wavelength of light to the characteristic feature size. In the ray-optical regime the wavelength is much smaller than the characteristic feature size. In this case, the simplification of geometrical optics can be applied and light propagation can be described as a geometrical propagation of rays. In the wave-optical regime, the wavelength is of the same order of magnitude than the feature size. In this case Maxwell’s equations have to be fully considered. For the third regime, where the wavelength is significantly larger than the feature size, structures can be approximated by homogenous effective media. In order to prevent any misunderstandings: The underlying physics is fully given by Maxwell’s
equations for all three optical regimes. Regime 1 and 3 just allow certain approximations that enable for example a more intuitive understanding, or shorter calculation times, when running optical models numerically.

![Figure 4: The three optical regimes for the interaction of light with an interface: subwavelength regime (a), where effective medium approaches can be applied, wavelength regime (b), where wave optics have to be applied, and the regime of geometrical optics for structures significantly larger than the wavelength (c).](image)

Important for this work is also Snell’s law for refraction at a planar interface and Fresnel’s equations to calculate reflectance and transmittance at a planar interface. Both can be found in standard optics textbooks. The grating equation (eq. (8)) allows for a reasonable understanding of the optics of a grating. It can be understood as a momentum conservation equation. Diffraction in this terminology means, that an arbitrary reciprocal lattice vector $K_{pq}$ of the grating is added to the grating parallel component of the incident wave vector $k_{inc,xy}$

$$k_{pq,xy} = k_{inc,xy} + K_{pq},$$

resulting in the parallel component of the diffracted wave vector $k_{pq,xy}$. The corresponding $z$-component of the diffracted wave vector can then be determined by the conservation of energy:

$$k_{pq,z} = \sqrt{\left(\frac{2\pi}{\lambda}\right)^2 - \left|k_{pq,xy}\right|^2}.$$  

The polar angle $\theta$ of the diffracted orders is then given by

$$\theta_{pq} = \arccos\left(\frac{k_{pq,z}}{2\pi / \lambda}\right).$$

Often it is also useful to determine the maximum number of propagating orders. A mode given by its indices $p$ and $q$ can propagate in the far field, if $k_{pq,z}$ (equation (9)) is real. For a simple grating with a periodicity of $A$ in only one direction, the maximum number of propagating orders is given by

$$m_{max} = \frac{A}{\lambda}.$$  

Note that $\lambda$ denotes the wavelength in the medium under consideration.
2.4.2 Antireflection structures

As seen in Figure 1, crystalline silicon has a high refractive index. According to Fresnel’s equations, the transition of light from one medium to another medium leads to reflection. The high refractive index contrast between air and silicon leads to a surface reflectivity of about 35%. Figure 5 shows the surface reflectivity at an air-Si interface. Weighted with the AM 1.5g spectrum, a solar cell without any antireflection structure would lose 16.3 mA/cm² due to front surface reflectivity for normal incident light. A simple antireflection coating (ARC) can reduce the reflectivity significantly. It works by destructive interference of reflected waves at the air-ARC interface and the ARC-Si interface. In order to reach destructive interference, the thickness $d_{ARC}$ has to be $\lambda_{Design}/4$ and the refractive index $n_{ARC}$ has to be $\sqrt{n_1n_2}$, when $n_1$ and $n_2$ are the refractive indices of the two media. The ARC should feature no absorption. For silicon solar cells the design wavelength usually is chosen in the range where the most photons in the AM 1.5g spectrum are incident (around 600 nm). There is no material available that fulfills the condition for the refractive index over the whole spectral range. The industrial standard ARC is SiN$_x$ [24], a good compromise between high refractive index and low absorption (and good surface passivation). For 75 nm of SiN$_x$ the reflectance curve is depicted in Figure 5 and the current density lost due to surface reflectance can be reduced to 4.8 mA/cm². By using additional ARC layers, the reflectivity can be further decreased. In high-efficiency silicon solar cells often a double layer antireflection coating (DARC) of SiN$_x$ and MgF$_2$ is used (e.g. [25]). Using a typical DARC the reflectivity loss can be reduced to 4.0 mA/cm². It can be seen, that planar ARC layers can reduce the reflectivity significantly, but especially in the blue wavelength range, where the refractive index of silicon increases strongly, planar ARC systems cannot fully suppress the front reflection losses. A detailed study of planar ARC systems with technologically available materials is presented in section 4.1.

![Graph](https://example.com/graph.png)

Figure 5: Reflectance at an air-Si interface with different antireflection structures. Calculations performed with OPAL 2 on PV-Lighthouse [26].
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In addition to planar layer systems also structured surfaces can be utilized to reduce surface reflectance. Typical is a pyramidally structured surface utilizing the intersecting 111-planes in crystalline silicon. Incident light that is reflected at the first interaction hits the air-Si interface a second time. Thus the reflectivity can be reduced to 4.4 mA/cm$^2$ (without ARC) and 0.9 mA/cm$^2$ (with ARC) in terms of reflected current density. An exemplary SEM picture indicating also the working principle is depicted in Figure 6. There is a variety of pyramidal textures. Most important are regular inverted pyramids (regular in size and arrangement, air pyramids in silicon with the tip to the bottom) and random upright pyramids (random size distribution, silicon pyramids in air with the tip to the top). A very detailed analysis of pyramidal textures and their optical properties can be found in [27,28]. Pyramids are the standard for industrial monocrystalline silicon solar cells, since they can be produced quite easily with KOH- or NaOH-based etching solutions. For multicrystalline silicon, where the 111-planes are oriented differently in each grain, isotextures are fabricated by acidic isotropic etching. These textures are not used within this work.

Figure 6: Pyramidal front side texture. The indicated light paths show that light reflected at the first interaction hits the opposite facet and can be coupled into the silicon at this second interaction. Even further interactions are possible and reduce the reflectance.

Beyond planar ARC systems and pyramids, there are also various kinds of nanostructures described in literature that can reduce the front surface reflectivity [29–33]. One promising approach that is also further investigated within this work is so called black silicon, a needle-like nanostructure. The basic principle why these nanostructures can reduce the surface reflectivity are mainly based on the so called moth eye effect. This effect was first described in [29]. Black silicon and its optical properties are investigated in detail in section 4.2.

2.4.3 Light trapping concepts

Beyond surface reflectance, there are also losses due to the low absorption coefficient of crystalline silicon in the NIR. Figure 7 shows the absorptance in crystalline silicon in dependence of the optical path length within the silicon. As the range of the depicted optical path lengths is of the order of magnitude of typical solar cell thicknesses, the light path length within the solar cell has to be enhanced, which can be done by internal reflections and by transferring light into oblique angles.
Figure 7: Absorbed photon flux after different optical path lengths in silicon. The grey area indicates the complete AM1.5 spectrum, the colored areas the absorbed photons.

This requires a texturing of the front and/or the rear of the solar cell. The pyramidal structures presented in section 2.4.2 for the purpose of antireflection also lead to a light path length enhancement. A pyramidal front surface in combination with a quasi-planar rear mirror is the current standard for industrial and also high-efficiency monocrystalline silicon solar cells [27,34,35]. For multicrystalline silicon, instead of pyramids, isotextures are used [36]. As an alternative to such standard front textures with feature sizes in the range of several micrometers, light path length enhancing structures at the rear have been investigated by several groups and show promising optical properties. Götzberger suggested 1981 the use of a Lambertian rear surface [37] and Tiedje and Yablonovitch deduced a limit for such Lambertian light trapping [38,39] that will be discussed in the next section. Heine and Morf, instead, suggested the use of diffractive structures at the rear [7,40] and demonstrated possible light path length enhancements up to a factor of five due to gratings. While numerous works investigated scattering or diffractive light trapping structures for thin film silicon solar cells, both, theoretically [41–46] and on final device level ([47–51]), many works aiming at the integration of diffractive rear structures into wafer-based crystalline silicon solar cells focused on theoretical investigations and optical measurements (e.g. [52–58]). Some typical light trapping structures used or described in literature are depicted in Figure 8.
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Figure 8: Sketch of different light trapping concepts. (a) depicts the widely used combination of pyramids at the front and a planar rear. (b) shows a planar front surface in combination with a diffuse Lambertian rear as suggested by Götzberger [37]. In this case only the light scattered into the loss cone (red area) can be coupled out at the subsequent interaction at the front. (c) refers to all concepts with diffractive gratings at the rear. In (d) front and rear textures are combined. When both sides are textured, there is no simple loss cone consideration possible.

2.4.4 Light trapping limits

There are several approaches to calculate a benchmark or limit for light trapping in crystalline silicon solar cells. While Shockley and Queisser in their first detailed balance analysis assumed an absorptivity of one up to the bandgap as an upper limit, later works introduced more detailed concepts about light trapping limits. The probably most famous and influential one, being the work of Yablonovitch [38,59] and Tiedje [39]. Using thermodynamical as well as detailed balance arguments they deduced a maximum light path length enhancement when light is totally randomized within a textured sheet. In the following a short derivation of this limit is given following the arguments in [38].

2.4.4.1 The Yablonovitch or Lambertian limit

We assume a textured sheet of a material with refractive index $n$ and incident light with irradiance $I_{\text{inc}}$ [W/m$^2$]. Due to surface textures at the front and/or rear, the direction of light propagation inside the sheet is totally randomized. This is especially the case if one texture is a perfect Lambertian scatterer. Such a Lambertian scatterer scatters light independently of the incident angle into all solid angles with a $\cos(\theta)$ characteristic (to avoid confusion: A plane Lambertian scatterer observed by the human eye or by a detector looks equally bright from all directions. This is not in contradiction with the $\cos(\theta)$ factor, because the observed area increases by $1/\cos(\theta)$ for oblique angles of observation). The scattering leads to a constant internal intensity $B_{\text{int}}$ [W/(m$^2$ sr)] and an internal irradiance $I_{\text{int}}$ [W/m$^2$] of
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\[ I_{in} = 2 \int B_{in} \cos \theta d\Omega = 2 \int_{0}^{\pi/2} \int_{0}^{2\pi} B_{in} \cos \theta \sin \theta d\theta d\varphi = 2\pi B_{in}, \tag{12} \]

where \( \Omega \) denotes the complete half space. The factor of 2 arises from the fact that light within the sheet propagates upwards and downwards with equal intensity (bidirectional).

The irradiance that can escape the structure is limited due to a restricted loss-cone and is given by

\[ I_{esc} = 2 \int_{0}^{\theta} \int_{0}^{2\pi} B_{in} T_{esc}(\theta) \cos \theta \sin \theta d\theta d\varphi = 2I_{in} \int_{0}^{\theta} T_{esc}(\theta) \cos \theta \sin \theta d\theta = I_{in} \frac{T_{esc}}{n^2}, \tag{13} \]

where \( T_{esc}(\theta) \) is the transmittance for light escaping. In the last step, instead of an angular dependent transmittance, an averaged transmittance \( \overline{T_{esc}} \) was used and the integral was evaluated. Again, a factor of 2 appears that indicates that light can leave the sheet on both sides within the loss cone.

The basic idea of the Yablonovitch limit is a detailed balance calculation: The amount of light entering the sheet must equal the amount of light escaping (without considering absorption):

\[ T_{in}(\theta)I_{in} = I_{in} \frac{T_{esc}}{n^2} \quad \text{or} \quad I_{in} = n^2 I_{in} \frac{T_{esc}(\theta)}{T_{esc}}. \tag{14} \]

This means, that the internal intensity is higher by a factor of \( n^2 \) assuming Lambertian scattering within the sheet when the transmission factors are equal. If a perfectly reflecting rear surface is considered, the intensity enhancement is increased to a factor of \( 2n^2 \) because the escape loss is reduced by a factor of 2. From now on we assume this situation: illumination from the front side and escape loss also only at the front side. If the textured sheet with a rear reflector absorbs a certain fraction of the incident light, an additional term has to be added to the right hand side of the detailed balance equation (14):

\[ T_{in}(\theta)I_{in} = I_{in} \frac{T_{esc}}{2n^2} + 2\alpha \omega I_{in} \quad \text{or} \quad I_{in} = \frac{I_{in} T_{esc}(\theta)}{\frac{T_{esc}}{2n^2} + 2\alpha \omega}, \tag{15} \]

where the absorption has been approximated using the first expansion term of the exponential function of Lambert-Beer’s law by \( 2\alpha \omega I_{in} \). This factor of 2 is caused by the fact, that the mean path length within the sheet is not \( w \) but \( \int_{-\pi/2}^{\pi/2} \frac{w}{\pi} \cos \theta \sin \theta d\theta = 2w \). Equation (15) indicates that the irradiance enhancement within the sheet is smaller when absorption is included. The absorption term in eq. (15) can now be written as:
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\[ A = 2 \alpha w I_{\text{tot}} = \frac{2\alpha w I_{\text{inc}} T_{\text{esc}}(\theta)}{T_{\text{esc}}^2 + 2\alpha w}. \]  

(16)

For very low absorption coefficients, the second term in the denominator can be neglected, which leads for equal transmission factors to \( A = 4n^2\alpha w \). This is \( 4n^2 \) times more compared to a single path through the cell \( A_{\text{single path}} = 1 - \exp(-\alpha w) \propto \alpha w \). Due to this \( 4n^2 \) factor, the Yablonovitch limit is often also denoted as \( 4n^2 \)-limit. However, this term should be used carefully as it holds only for very weak absorption. In Figure 9 the absorptance calculated according to \( A = 1 - \exp(4n^2\alpha w) \) and equation (16) are compared and it can be seen, that for crystalline silicon there is a significant difference and equation (16) should be used. One further remark: The Yablonovitch limit is not an actual upper limit, it gives just the absorptance that can be reached using structures randomizing the light paths. Structures exceeding this “limit” for certain wavelengths are possible and have been reported for special cases [60–62]. However, the thermodynamical arguments of Yablonovitch indicate, that it is not possible to exceed the limit over a broad spectral range. Structures that are well designed for a specific wavelength will perform below this limit in other spectral ranges.

2.4.4.2 Lambertian light trapping analyzed by Götzberger

Already one year before Yablonovitch’s work, Götzberger presented an absorption calculation for silicon solar cells with a Lambertian scatterer at the rear side [37]. By a very similar consideration, he deduced that, when light enters the cell at the front side with a transmission factor of one and is scattered by a Lambertian rear, a fraction of \( 1/n^2 \) of the incident light is scattered into the loss cone while the rest is totally internally reflected at the planar front surface. By using the geometric series and separating light absorbed within and outside the loss cone, a total absorptance can be calculated:

\[ A = \frac{\exp(-\alpha w)R \left(1 - \frac{1}{n^2} - 2G\right)}{1 - 2RG} + (1 - \exp(-\alpha w)) \left(1 + \frac{\exp(-\alpha w)R}{n^2(1 - 2RG)}\right), \]  

(17)

with

\[ G = \frac{1}{\pi} \int_{\pi}^{\pi/2} \sin \varphi \cos \varphi \exp \left(\frac{-2\alpha w}{\cos \varphi}\right) d\varphi. \]  

(18)

Calculating the absorptance according to equation (17) numerically leads to the results depicted in Figure 9, where also the Yablonovitch limit is plotted. Obviously, these two considerations lead to very similar results, which can also be shown analytically using weak absorption approximations as also considered by Yablonovitch.
2.4.4.3 Lambertian light trapping analyzed by Green

In addition to Götzberger and Yablonovitch, also Green in detail considered different configurations of light trapping structures containing Lambertian surfaces [63]. He deduces (exact) analytical results similar to the approach of Götzberger and also a formula valid in the weak absorption case:

$$A = \frac{1 - \exp(-4\alpha w)}{1 - \exp(-4\alpha w) + \frac{1}{n} \exp(-4\alpha w)}.$$  \hspace{1cm} (19)

The result for this formula for a 200 µm thick silicon solar cell is also added to Figure 9. All three approaches (Yablonovitch, Götzberger and Green) lead to very similar results. Due to its widest use in literature, in the following work equation (16) by Yablonovitch will be used as reference system for Lambertian light trapping.

![Figure 9: Comparison of different light trapping limits considering Lambertian light trapping.](image)

2.4.5 Parasitic absorption

In an actual solar cell, light can be absorbed not only in the active silicon bulk generating electron hole pairs, but also parasitic absorption occurs. In a typical solar cell important parasitic absorption losses comprise absorption in the front metal grid, absorption in the rear side metallization, absorption in the antireflection coating and also free carrier absorption within the Si. All of these parasitic absorption mechanisms reduce the useful absorption and thus \( J_{SC} \). In the following the individual parasitic mechanisms important for this work are described briefly. Parasitic metal absorption occurs at the front side grid and at the rear side metallization. The area fraction covered by the front side grid should be as small as possible to reduce reflection anyway. The rear side metal absorption can be reduced by adding a dielectric buffer layer between silicon and metal as in the PERC concept. For structured interfaces between dielectrics and metals the excitation of surface plasmon polaritons strongly increases and therefore structured metal interfaces have to be avoided or at least shielded by buffer layers. This is especially relevant for novel light trapping structures featuring structured interfaces at
the rear side. Absorption in the antireflection coating is especially important in the short wavelength range, where the typical materials like SiNx slightly absorb light. Therefore ARCs have to be optimized with a trade-off between avoiding parasitic absorption and reaching high refractive indices, which will be discussed in detail in section 4.1. Free carrier absorption (FCA) within the silicon occurs, when an already excited charge carrier absorbs a photon and is lifted into a higher excited state within the same band. The excitation energy subsequently gets lost to phonons. FCA increases with increasing wavelength and strongly depends on the density of free charge carriers $n$ and $p$ and thus on the doping level in Si. Therefore it plays an important role in highly doped regions like the emitter or in the back surface field, but also in any additional structure containing free charge carriers (for example transparent conductive oxides etc.). FCA has been parameterized for the wavelength range of 1.0-2.0 $\mu$m in dependence of the doping type and level by Ruediger et al. [64]. The absorption coefficients for n- and p-type doping are given by:

$$\alpha_{\text{FCA},p} / \text{cm}^{-1} = 2.6 \cdot 10^{-18} \left( \lambda / \mu\text{m} \right)^{2.4} / \text{cm}^{-3},$$

(20)

$$\alpha_{\text{FCA},n} / \text{cm}^{-1} = 1.8 \cdot 10^{-18} \left( \lambda / \mu\text{m} \right)^{2.6} / \text{cm}^{-3}.$$  

(21)

### 2.5 Electrically planar but optically structured solar cells

Combining the fundamentals described in sections 2.2, 2.3, 2.4., the overall question is: What is the best solar cell structure with regard to light trapping but also with regard to the cell’s electrical properties? A highly efficient solar cell requires efficient light trapping, but at the same time excellent surface passivation and very good electrical contacts. This work concentrates on light trapping, but while doing this, all other aspects are considered thoroughly to avoid an improvement of one single property (e.g. near infrared EQE) while deteriorating other properties (e.g. $V_{OC}$ or FF). One concept that potentially fulfills these requirements is an electrically flat, but optically structured solar cell. This means that the cell has electrically planar interfaces that are well passivated and additional optical structures that enable light trapping and make the surfaces optically rough. We call this concept EPOS (electrically planar, optically structured). The fundamental limit that can be reached with a single junction silicon cell has been already described by Shockley and Queisser [3]. Recently, Richter et. al reassessed this limit including Auger recombination and novel parameterizations for silicon material data [4]. Assuming Lambertian light trapping, undoped bulk material and perfectly passivated surfaces, they showed that the optimum cell thickness is approximately 100 $\mu$m. Aiming at highest efficiencies, this is what we need to target: Lambertian light trapping in a 100 $\mu$m thin wafer combined with excellent surface passivation and low bulk doping. The following work wants to contribute a few small steps and ideas pointing into this direction.
3 Methods for the optical simulation of light trapping in solar cells

Within this chapter, I present methods for the optical simulation of various structures in silicon solar cells for light trapping. The transfer matrix method (TMM), which is used for planar layer systems, is briefly introduced in 3.1.1. For the simulation of gratings, which are central for this thesis, the wave optical simulation method RCWA (rigorous coupled wave analysis) is presented in 3.1.2. A short introduction of ray tracing and existing methods to combine different methods is given in 3.1.3 and 3.1.4. The combination of various front and rear structures requires an efficient combination of different simulation techniques. Thus, in Section 3.2 I introduce the new simulation formalism OPTOS (Optical Properties of Textured Optical Sheets), which I developed together with Nico Tucher who conducted his dissertation in parallel to this work [65]. OPTOS allows for an efficient calculation of textured optical sheets with arbitrary interface structures.

3.1 Used standard methods

3.1.1 Transfer matrix method

The transfer matrix method (TMM) efficiently calculates the propagation of coherent electromagnetic waves in planar layer systems. The following short description as well as the TMM implementations used in this work are based on [66] and this description can also be found in [67]. The method is based on a description of a single planar layer by a characteristic 2x2 matrix:

\[
\begin{bmatrix}
E_a \\
H_a
\end{bmatrix} =
\begin{bmatrix}
\cos \delta & i \sin \delta / \eta \\
i \eta \sin \delta & \cos \delta
\end{bmatrix}
\begin{bmatrix}
E_b \\
H_b
\end{bmatrix},
\]

where \(E_a\) and \(H_a\) denote the electric and the magnetic field at the first interface and \(E_b\) and \(H_b\) the fields at the second interface. The phase factor \(\delta\) is given by:

\[
\delta = \frac{2 \pi \cdot N \cdot d \cdot \cos \theta}{\lambda},
\]

with the complex refractive index \(N\), the layer thickness \(d\) and the polar angle \(\theta\). \(\eta\) is the optical admittance, depending on the polarization of the incident light.
3 Methods for the optical simulation of light trapping in solar cells

\[ \eta_{TE} = \sqrt{\frac{\varepsilon_0}{\mu_0}} N \cos \theta \quad \eta_{TM} = \sqrt{\frac{\varepsilon_0}{\mu_0}} \frac{1}{\cos \theta}, \quad (24) \]

For a multi-layer system containing \( q \) individual films, each film is described by a characteristic matrix as in eq. (22) and the effect of the complete multi-layer system is given by the product of all the individual matrices:

\[ \begin{bmatrix} B \\ C \end{bmatrix} := \left( \prod_{r=1}^{q} \begin{bmatrix} \cos \delta_r & i \sin \delta_r / \eta_r \\ i \eta_r \sin \delta_r & \cos \delta_r \end{bmatrix} \right) \begin{bmatrix} 1 \\ \eta_m \end{bmatrix}, \quad (25) \]

While all layers and the substrate may feature arbitrary complex refractive indices, the method is restricted to absorption-free incident media. Using the quantities B and C, reflectance, transmittance and absorptance can be calculated:

\[ R = \left| \frac{\eta_0 B - C}{\eta_0 B + C} \right|^2 \quad T = \frac{4\eta_0 \text{Re}(\eta_m)}{|\eta_0 B + C|^2} \quad A = 1 - R - T. \quad (26) \]

There are various implementations of this set of formulas available. For most calculations within this work, a Matlab-based implementation was used. For quick tests and an intuitive understanding the program RAT, developed at Fraunhofer ISE, offers an implementation including a graphical user interface [68].

### 3.1.2 Rigorous coupled wave analysis (RCWA)

The rigorous coupled wave analysis is a method designed for determining the optical properties of diffractive structures. For a full deduction and description of the method, see the works of Gaylord [69,70], Moharam [71–73] and Li [74,75]. Here, the method and its most important properties are sketched briefly. A good description can also be found in [67].

![Figure 10: Sketch of an arbitrary grating with a periodicity in the x-direction. Region I and III are homogenous media (substrate and superstrate) and region II features a periodic modulation of the refractive index.](image-url)
The RCWA offers a numerical solution of Maxwell’s equations for a system as depicted in Figure 10. Region I and III are homogeneous media and region II features a periodic modulation of the refractive index. It can be separated into thin individual layers with respect to the \(z\)-direction in order to avoid any \(z\)-dependence within one layer. The mathematical formulation of the problem is to find solutions for the scalar Helmholtz equation and subsequently for the complete set of Maxwell’s equations. The basic idea is to express the solutions in region I and III as well as the structure in region II and its solutions by a Fourier expansion of plane waves. In a second step, all individual solutions are coupled by considering continuous boundary conditions. If an infinite amount of Fourier components is considered, the method leads to an exact result. In practice, the number of orders has to be truncated to avoid infinite calculation times. For a grating with a periodicity in one dimension, the calculation time scales with the number of Fourier modes to the power of three. Hence, the number of Fourier orders needed for a sufficiently precise result has to be carefully evaluated by convergence analyses. The maximum number of orders that can propagate is given by \(m_{\text{max}} = \Lambda / \lambda\) (see equation (11)) and is an absolutely lower limit for the number of Fourier orders that have to be considered. In most cases additional evanescent modes have to be considered for a precise solution.

There are several implementations of the RCWA available. For all simulations in this work an implementation by Lalanne called “Reticolo Code 2D” [76,77] has been used.

3.1.3 Ray tracing

Ray tracing is the most commonly used optical simulation method for silicon solar cells, as the structure size for the most widely used surface textures, pyramids or isotextures, is usually in the range of several \(\mu\)m and thus significantly larger than the wavelengths of interest. Brendel et al. for example introduced the ray tracing program Sunrays specifically designed for photovoltaic applications [78]. The widely used simulation software Sentaurus Device also contains a ray tracer to generate optical result files as input for electrical solar cell simulations (e.g. [79]). Also the platform PV Lighthouse offers versatile ray tracing solutions for typical large scale solar cell textures [80]. Within this work, also the in-house ray tracing tool Raytrace3D [81,82] has been used to generate matrices for the formalism OPTOS that is introduced in the following section 3.2. As the ray tracing itself is not in the focus of this work, only general and very simplified remarks follow here.

Ray tracing is the solution to a mainly geometrical problem: the interaction of light rays with a specific geometry of media with certain optical properties. Most methods follow a so called Monte Carlo approach. A large number of rays is traced and each ray terminates at a certain point in a certain detector or gets lost. By averaging over all individual rays, the final result, e.g. reflectance, transmittance or absorptance, can be approximated. Thus the number of used rays is a crucial parameter for convergence and also for the numerical calculation effort. In addition to the mere geometry, there are certain properties that can be attributed to a light ray, for example polarization,
which is a concept actually based on wave optics. In a similar way, the transfer matrix method described in section 3.1.1 can be included to enable the simulation of antireflection coatings for example, which cannot be described by pure ray optics. While this includes some wave optical concepts into ray tracing one should keep in mind that the light propagation is still governed only by the geometry and important wave optical quantities like the phase are neglected. Thus, for each structure it has to be carefully evaluated if this is a valid approximation.

### 3.1.4 Combinations of wave optical and ray optical methods

As introduced in 2.4.3, combining surface structures at the front for antireflection with surface structures at the rear for enhanced light trapping might be a promising approach to reach highest currents. The combination of such surface structures within one simulation framework was a key challenge within this work. If front and rear of a solar cell are textured with structures operating in different optical regimes, for example pyramids at the front that are significantly larger than the wavelength and a diffractive grating with a period in the range of the wavelength at the rear, there are different options for solving this problem. The first option is a fully wave optical modeling, which has several drawbacks. As already indicated, the numerical effort increases significantly with increasing periods. For three dimensional surface textures in silicon, already for periods of a few µm calculations are not feasible with respect to storage and calculation time. Furthermore, a fully coherent wave optical description produces interference effects, e.g. in thick layers, that are not relevant for solar cells – either due to slight deviations in the sample or light path geometry or due to the finite coherence of the used light. Such interference effects in principal can be smoothed out by clever algorithms averaging for example over a small wavelength or thickness range. However, this averaging is not trivial and always remains a source of uncertainty. A second and more preferable option is the combination of different simulation methods optimized for the respective optical regimes within one simulation framework.

One approach is to use ray tracing as fundamental method but to include surface interactions not governed by geometrical optics. This can be realized by using pre-calculated lookup tables or bidirectional reflectance distribution functions at certain interfaces that have been determined with another method, e.g. a wave optical simulation method, or by a separate calculation that is started when a light ray hits the corresponding interface.

For the special case of silicon solar cells with pyramidal front textures and diffractive gratings at the rear, Wellenzohn and Hainberger presented a 2D ray tracing method including RCWA [83]. Rothemund et al. extended this approach to 3D ray tracing, but still used only binary line gratings at the rear [58]. These methods are very flexible and in principal capable of calculating the optical properties of the light trapping structures developed and investigated within this work. In the following section, I introduce an alternative, matrix based method, which has several advantages compared to ray tracing approaches including wave optics.
3.2 Development of the simulation formalism OPTOS

To overcome the limitations of the previously described simulation techniques, we developed the simulation formalism OPTOS (Optical Properties of Textured Optical Sheets). Basically, OPTOS is aiming for the calculation of the optical properties of an absorber with two arbitrary surface textures with comparatively low computational effort. The angular space is discretized into a finite set of angle channels. The occurring light path directions are binned to the previously defined angle channels. Surface interactions as well as light propagation inside the textured optical sheet are simulated only for this discrete set of angles. This allows for a description of every surface by means of redistribution matrices for transmission and reflection that are specific to a surface and need to be calculated only once for a specific surface or interface. These matrices describe the redistribution of light between the pre-assigned discrete angle channels. The results for redistribution at the front and the rear are then coupled non-coherently using a propagation matrix that accounts for the light propagating through the absorber. Thereby, reflection, absorption, transmission and also a one-dimensional absorption profile of a sheet with arbitrary surface textures can be obtained via matrix multiplications. Together with Nico Tucher, I introduced the basics of the OPTOS method in three joint publications [84–86].

3.2.1 Related methods from literature

There is one important method that was introduced by Mellor et al. [54,87], which inspired the OPTOS development and bears some resemblance to OPTOS for the special case of a sheet with one planar interface and one grating interface. In such a sheet, a grating produces a finite set of diffraction orders according to the grating equation (8). As the second interface is planar and specularly reflects light, this finite set is preserved in all subsequent interactions. Mellor described this finite set of propagating modes with the means of vectors and matrices. OPTOS, as described in the following sections, overcomes the restriction to such special systems, but uses similar matrices and a similar formalism to deduce the optical properties based on these matrices. The method introduced by Mellor (in the following referred to as Mellor method) can be used as reference method for the named systems.

Shortly after the publication of OPTOS [84], Li et al. published a very similar formalism based on very similar concepts and ideas [88]. As this formalism, called “angular matrix framework” was not known at the time of the OPTOS development, it is not further discussed here but just mentioned as related method.

3.2.2 Basic mathematical formulation of OPTOS for 2D systems

The following description is mainly based on the first OPTOS publication [84]. For the sake of simplicity within this chapter the basic mathematical formulation of OPTOS is presented for only two-dimensional systems. This means that all these systems can be described within the \(x-z\)-plane (and could be infinitely extended in the third dimension without any \(y\)-dependence) and directions of light
propagation can be fully described by the polar angle $\theta$. In order to allow for using a matrix and vector based description of light propagation, the angle space is divided into discrete angle channels. The power distribution inside the textured sheet can therefore be represented by a power distribution vector with discrete elements. Each element contains the power fraction $p(\theta)$ distributed into a certain angular range specified by a polar angle $\theta$.

$$v = \begin{pmatrix} p(\theta_1) \\ p(\theta_2) \\ \vdots \\ p(\theta_n) \end{pmatrix}. \quad (27)$$

The non-coherent (as the vector contains only power values, no phase information) propagation of light within a homogeneous medium can then be represented by multiplication of a propagation matrix with this vector. As propagation of light in a homogeneous medium does not change the direction of light propagation, but may reduce the power in the different channels according to Lambert-Beer’s law, the propagation matrix features non-zero elements only on its diagonal.

$$D = \begin{pmatrix} e^{-\alpha d \cos \theta_1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & e^{-\alpha d \cos \theta_n} \end{pmatrix}. \quad (28)$$

In this matrix, $\alpha$ is the absorption coefficient, $d$ the thickness of the optical sheet and $\theta_i$ the polar angle of the respective angle channel. As well as the propagation of light, also the surface interaction can be represented by the multiplication of a matrix with the vector $v$. Such a surface interaction may redistribute light from each angle channel to other angle channels and therefore the corresponding redistribution matrix may also have off-diagonal non-zero elements. For reflection as well as for transmission such a redistribution matrix can be defined.

$$R, T = \begin{pmatrix} \theta_1 \rightarrow \theta_1 & \cdots & \theta_1 \rightarrow \theta_i \\ \theta_2 \rightarrow \theta_2 & \cdots & \theta_2 \rightarrow \theta_i \\ \vdots & \ddots & \vdots \\ \theta_n \rightarrow \theta_n & \cdots & \theta_n \rightarrow \theta_i \end{pmatrix}, \quad (29)$$

where $R$ denotes a reflection matrix and $T$ a transmission matrix. A very important property of such matrices is the fact that the column sum has to be smaller than or equal to one, which corresponds to the conservation of energy. If the column sum of a reflection matrix, for example, is one, this means that all light is reflected at the interface, which implies no transmission and no absorption at the interface. The matrix in this case is called stochastic.

Given the propagation and redistribution matrices for an exemplary sheet with two interfaces (denoted by subscripts “1” and “2”) as depicted in Figure 11, the evolution of the light distribution given by
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vector $v$ can be calculated step by step. Each interface is characterized by four matrices: reflection and transmission matrix for light incident from above and below the interface (denoted by the superscript “down” or “up”), respectively.

*Figure 11: Light propagation in a continuous medium with textured surfaces on both sides. Incoming light is divided by reflection and transmission into different channels as depicted in (a). (b) focuses on the power distribution vectors inside the sheet. The power fractions after entering through the front surface are described by $v_0'$. Before the interaction at the rear side it is called $v_1$, after reflection $v_1'$ and so on. The bulk propagation, where no redistribution but only absorption occurs, is described by the propagation matrix $D$.

After having calculated all redistribution matrices with appropriate methods, there are two different ways of calculating all the relevant information for such a system. The first is fully matrix based, the second can be called vector based. While the first one provides the more compact mathematical formulation, the second one allows for a higher level of insight into the light propagation and features advantages with respect to the numerical implementation. Both approaches are mathematically equivalent, just the technical way of the numerical calculation is different.

**Matrix based approach**

Given the naming convention of Figure 11(a), an absorption, reflection and transmission matrix for the complete system can be calculated. As for example the reflection of the complete system is composed of different contributions, the corresponding matrices can be summed up to get the system matrices.

More precisely, the overall reflection is the sum of primary surface reflection ($R_{down}^1$) and escape reflection. The escape reflection requires transmission at the front interface first ($T_{down}^2$), the propagation to the rear ($D$), reflection at the rear side ($R_{down}^2$) and again propagation to the front ($D$).

Then, an arbitrary number of further cycles is possible (term in square brackets in equation 30) before the light has to be coupled out again ($T_{up}^2$). For the absorption, the formula is more complicated as upwards and downwards propagating light has to be separated. The formula for absorption can be understood more easily in the vector based approach described below. The transmission can be understood similar to the reflection: At first transmission through the front surface is required ($T_{down}^2$), then propagation to the rear ($D$), then an arbitrary number of cycles through the sheet and finally downwards transmission through the rear interface ($T_{down}^3$).
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\[ R = R_{2\downarrow}^{\text{down}} + T_{2\uparrow}^{\text{up}} \left[ \sum_{i=0}^{\infty} (DR_{\downarrow}^{\text{down}} DR_{\uparrow}^{\text{up}})^i \right] DR_{\downarrow}^{\text{down}} DT_{2\downarrow}^{\text{down}}, \]  
\( (30) \)

\[ A = \left[ \sum_{i=0}^{\infty} (R_{\uparrow}^{\text{up}} DR_{\downarrow}^{\text{down}})^i D + \sum_{i=0}^{\infty} (R_{\downarrow}^{\text{down}} DR_{\uparrow}^{\text{up}})^i D - \sum_{i=0}^{\infty} (DR_{\downarrow}^{\text{down}} DR_{\uparrow}^{\text{up}})^i DR_{\downarrow}^{\text{down}} D \right] T_{2\downarrow}^{\text{down}}, \]  
\( (31) \)

\[ T = T_{1\downarrow}^{\text{down}} \left[ \sum_{i=0}^{\infty} (DR_{\downarrow}^{\text{down}})^i \right] DT_{2\downarrow}^{\text{down}}. \]  
\( (32) \)

Conservation of energy leads to the fact that for all redistribution matrices \( \|R\| \leq 1, \|T\| \leq 1 \) with respect to the column-sum norm, whereas for an absorption coefficient \( \alpha > 0 \) \( \|D\| < 1 \). This means, for a matrix \( X \), which is the result of multiplications between matrices \( D, R \) and \( T \), that the Neumann series (geometric series for matrices) \( \sum_{i=0}^{\infty} (X)^i \) converges to \((I - X)^{-1}\) [89], where \( I \) denotes the identity matrix. Instead of one infinite sum, which has of course to be truncated at some \( i_{\text{max}} \), for this geometric series approach only four matrices have to be multiplied and the resulting matrix has to be inverted. The result is exact with respect to the included number of system passes and corresponds to the iterative approach for the limit of \( i_{\text{max}} \to \infty \). This accessibility of the “exact” result enables a meaningful convergence analyses.

\[ R = R_{2\downarrow}^{\text{down}} + T_{2\uparrow}^{\text{up}} (I - DR_{\downarrow}^{\text{down}} DR_{\uparrow}^{\text{up}})^{-1} DR_{\downarrow}^{\text{down}} DT_{2\downarrow}^{\text{down}}, \]  
\( (33) \)

\[ A = \left[ (I - R_{\uparrow}^{\text{up}} DR_{\downarrow}^{\text{down}})^{-1} (I - DR_{\downarrow}^{\text{down}} DR_{\uparrow}^{\text{up}})^{-1} D - (I - R_{\downarrow}^{\text{down}} DR_{\uparrow}^{\text{up}})^{-1} (I - DR_{\downarrow}^{\text{down}} DR_{\uparrow}^{\text{up}})^{-1} R_{\downarrow}^{\text{down}} D \right] T_{2\downarrow}^{\text{down}} \]  
\( (34) \)

\[ T = T_{1\downarrow}^{\text{down}} (I - DR_{\downarrow}^{\text{down}})^{-1} DT_{2\downarrow}^{\text{down}}. \]  
\( (35) \)

The absorbance, reflectance and transmittance itself can then be calculated by multiplying these matrices with the incident power vector \( v_0 \) and summing over all resulting vector entries:

\[ R = \sum_j (R v_0)_j, \]  
\( (36) \)

\[ A = \sum_j (A v_0)_j, \]  
\( (37) \)

\[ T = \sum_j (T v_0)_j. \]  
\( (38) \)

**Vector based approach**

While the previously described approach yields a quite closed mathematical formulation, the vector based approach allows for a more intuitive understanding of the formalism. The involved matrices and
the vectors are identical, but instead of generating complete system matrices, the propagation and redistribution matrices are multiplied to the incident vector step by step. Thus, the power distribution vectors after all subsequent surface interactions (as depicted in Figure 11(b)) are calculated and the optical properties are deduced from these sets of vectors. As in the context of silicon solar cells the absorption within the silicon bulk is the most relevant quantity, the following description is restricted to the calculation of the absorption and uses $v_0^\text{down} = T_2^\text{down} v_0$ as a starting point.

As described above, the propagation through the optical sheet including the angle dependent absorption can be obtained by a multiplication of vector $v_0$ with the propagation matrix $D$. The power distribution at this point is described by the vector $v_1$. Similarly the reflection at the rear surface, the upward propagation and the subsequent front surface reflection can be described by matrix multiplications with matrices $R_1^\text{down}, D$ and $R_2^\text{up}$, respectively. This leads to the power distribution vector $v_2'$. The primed vector signs always indicate, that they describe the system directly after a surface interaction. In this notation all vectors $v$ can be calculated by the following matrix products starting from vector $v_0$. The remaining total power fraction $P_i$ can be obtained by summation over all vector entries. Note that this is not the sum over the index $i$, which is related to the path number.

$$v_{2j} = (R_2^\text{up} DR_1^\text{down} D)' v_0$$
$$v'_{2i+1} = (R_2^\text{up} DR_1^\text{down} D)' R_1^\text{down} D v_0$$
$$P_i = \sum_j (v_i)_j$$

The surface interaction and propagation with absorption can be repeated via multiplication of the corresponding matrices until no significant fraction of the incoming power is left in any channel. At this point all relevant information is contained in the power distribution vectors $v_i$ and $v_i'$. From these vectors, the quantities reflectance, absorptance and transmittance can be determined. In the following the exemplary determination of the absorptance $A$ is described. The absorbed fraction of incoming power $A$ is equal to the sum of the power loss during the transition of the optical sheet from the rear to the front surface, $A_{up}$, and from the front to the rear surface, $A_{down}$. The absorbed power fraction during such a transition is equal to the difference between the total power fraction at the beginning (directly after a surface interaction) and the total power fraction at the end of the path (directly before a surface interaction). The summation of all of these components leads to the total absorptance $A$.
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\[
A = A_{\text{down}} + A_{\text{up}} = \left( \sum_{i=0}^{i_{\text{max}}} (P'_{2i+1} - P_{2i+1}) \right) + \left( \sum_{i=0}^{i_{\text{max}}} (P'_{2i} - P_{2i}) \right),
\]

This iterative approach requires the calculation of the vectors \( v_i \) up to a certain path number \( i_{\text{max}} \). The required number \( i_{\text{max}} \) depends on the strength of absorption and escape losses. In weakly absorbing media that trap the light effectively, e. g. a cavity, \( i_{\text{max}} \) becomes very large. In this case, the iterative calculation can again be replaced by the mathematically more appropriate and elegant approach using the Neumann series. Note that this formula is basically the same than the combination of equation (34) and (37):

\[
A = P_e - P_i + P'_e - P'_i + P''_e - P''_i + \ldots
\]

\[
= \sum_i \left( \sum_{j=0}^{i_{\text{max}}} (R^e_{j}DR^e_{i-j})v_i' - \sum_{j=0}^{i_{\text{max}}} (R^i_{j}DR^i_{i-j})Dv_i' + \sum_{j=0}^{i_{\text{max}}} (R'^e_{j}DR'^e_{i-j})DR'^e_{i-j}Dv_i' \right)
\]

\[
= \sum_i \left( \sum_{j=0}^{i_{\text{max}}} (I - R^e_{j}DR^e_{i-j})v_i' - \sum_{j=0}^{i_{\text{max}}} (I - R^i_{j}DR^i_{i-j})Dv_i' + \sum_{j=0}^{i_{\text{max}}} (I - R'^e_{j}DR'^e_{i-j})DR'^e_{i-j}Dv_i' \right)
\]

The vector based calculation allows not only for the calculation of the absolute absorptance, but also of a one-dimensional cumulative absorption profile \( A(z) \). The cumulative absorption contains the information how much light is absorbed up to a depth \( z \). In addition to the vectors \( v_i \), also the \( z \)-dependent propagation matrix \( D(z) \) and a \( z \)-dependent absorption matrix \( A_{\text{down}}(z) \) is needed.

\[
D(z) = \begin{pmatrix}
1 & e^{-a/z/\cos \theta_i} & \ldots & 0 \\
\vdots & \ddots & \ddots & \vdots \\
0 & \ldots & e^{-a/z/\cos \theta_i} & 0
\end{pmatrix},
\]

\[
A_{\text{down}}(z) = \begin{pmatrix}
1 - e^{-a/z/\cos \theta_i} & \ldots & 0 \\
\vdots & \ddots & \vdots \\
0 & \ldots & 1 - e^{-a/z/\cos \theta_i}
\end{pmatrix},
\]

The absorption for upwards and downwards propagating light is again separated and depends also on \( z \). For the upwards propagating light, the path length starts at the rear, so the correct exponent is not \( z/\cos \theta_i \) but \( (d-z)/\cos \theta_i \). An additional absorption matrix \( A_{\text{up}}(z) \) has to be defined for upwards propagating light:

\[
A_{\text{up}}(z) = \begin{pmatrix}
1 - e^{-a(d-z)/\cos \theta_i} & \ldots & 0 \\
\vdots & \ddots & \vdots \\
0 & \ldots & 1 - e^{-a(d-z)/\cos \theta_i}
\end{pmatrix},
\]

The cumulative absorption for down- and upwards propagating light is then given by:

\[
A_{\text{down}}(z) = \sum_j \left( \sum_{i=0}^{i_{\text{max}}} A_{\text{down}}(z)v_i' \right)_j = \sum_j \left( A_{\text{down}}(z) \sum_{i=0}^{i_{\text{max}}} v_i' \right)_j,
\]

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\[
A_{\text{up}}(z) = \sum_j \left( \sum_{i=0}^{\text{max}} A_{\text{up}}(z) v_{2i+1} \right) = \sum_j \left( A_{\text{up}}(z) \sum_{i=0}^{\text{max}} v_{2i+1} \right),
\]

(46)

These two terms can be used to calculate the cumulative absorption profile giving the absorptance between the top surface \((z = 0)\) and the depth \(z\):

\[
A(z) = A_{\text{down}}(z) + A_{\text{up}}(0) - A_{\text{up}}(z),
\]

(47)

where \(A_{\text{down}}(z)\) describes the absorptance for downward propagating light between \(z = 0\) and \(z\), \(A_{\text{up}}(0)\) the total absorption for upward propagating light and \(A_{\text{up}}(z)\) the absorption for upward propagating light between \(z = d\) and \(z\). In the context of photovoltaics, a generation profile that is directly related to the absorption profile is of interest. It contains the information how many electron hole pairs are generated between a certain depth \(z\) and \(z + dz\) and is a common input parameter for electrical solar cell simulations. It may be calculated either by considering the absorbed amount of light according to the cumulative absorption profile in finite steps or by differentiating an interpolated cumulative absorption profile. [84]

**Considering polarization effects**

All matrices and vectors can be extended to incorporate polarization dependent entries. Each vector entry can be replaced by two entries: the first one containing the power fraction with TE polarization and the second one TM polarization. Accordingly, each matrix entry then has to be replaced by a 2x2 matrix representing the redistribution between TE and TM polarization. To get a result for unpolarized incident light, while simultaneously correctly tracing the independent directions of polarization during multiple surface interactions, one can perform two separate calculations for TE and TM incident light and average the results afterwards. [84]

**Angle Discretization**

The basic formulation of OPTOS as described within this section is completely independent of the actual angle discretization. As long as the same angle channels are used for all matrices, the formalism in principle works and as long as the discretization is fine enough results should converge to the result that is exact with regard to the angle discretization. However, to be able to combine various matrices, one “standard angle discretization” has to be defined. With regard to the polar angle, angle channels with equidistant \(\sin(\theta)\) values have been chosen (Figure 12a). The \(\sin(\theta)\)-values to be considered are in the range between 0 and 1. The latter corresponds to a polar angle of 90°, which corresponds to an infinitely large light path length. Therefore the polar angle of 90° is omitted and a discretization according to the following formula is chosen [84]:

\[
\sin(\theta) = \frac{2i}{2r-1},
\]

(48)
with \( r \) being the number of angle channels and the index \( i = 0, 1, \ldots, r - 1 \). The angles given by eq. (48) define the angle channel centers that are equally spaced in the \( \sin(\theta) \)-space. This corresponds to equally large projected lengths of the angle channels on the \( x \)-axis. Only the innermost angle channel from \( \sin(\theta_0) = 0 \) to \( \sin(\theta_r) \) is smaller. Figure 12 (a) illustrates the angle channels for an example value of \( r = 4 \). For actual calculations, \( r \)-values between 50 and 100 were found to be reasonable with respect to balancing calculation effort and inaccuracies due to a rough discretization (see also convergence analyses in Figure 25).

### 3.2.3 Basic mathematical formulation of OPTOS for 3D systems

Because many systems relevant to silicon solar cells feature surface textures, which can be described accurately only in three dimensions, OPTOS has been extended to 3D. The following description is mainly based on the second OPTOS publication [85]. The extension to 3D means that light can impinge interfaces from any direction of the full angle space. Note that there is still no information about the actual position of light-surface interactions and thus OPTOS – as in the 2D case – is tailored to sheets, with homogeneous in-plane properties. To consider 3D textures, the fundamental principle of the formalism (as expressed in formulas \((30)\) to \((47)\)) stays the same. However, an additional angle, the azimuth angle \( \delta \) is needed to describe the full angle space. In the following, the changes implied by this additional angle are presented without repeating the basic formulas.

#### Angle Discretization

Especially the discretization of the angular space has to be realized differently in 3D, because additionally the azimuth angle has to be discretized. Therefore, each polar angle channel (with a polar angle discretization as before in 2D) is divided into a certain number of equally large channels in a way that the projected area of all angle channels on the \( x \)-\( y \) plane is equally large [85]. This means, that the larger the polar angle, the higher is the number of different azimuth angles, because the solid angle corresponding to a polar angle range increases with increasing polar angle. Figure 12 (b,c,d) illustrates the chosen angle channels again for \( r = 4 \) and thus for a small total number of angle channels.
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Figure 12: Angle discretization for 2D (a) and 3D OPTOS (b,c,d). (a) shows the polar angle discretization based on equidistant $\sin(\theta)$-values. (b) shows the discretized surface of the three-dimensional half sphere and (c) its projection onto the x-y-plane. The discretization features angle channels with equally large projected areas in the x-y-plane and symmetry elements as highlighted in red and depicted in (d). The 45°-symmetry element is just one possible example and such elements can be used to reduce the number of calculations. (b,c,d) taken from [85].

This discretization leads to a linear relation between the polar angle interval index $i$ and the associated number of azimuth angle intervals for one symmetry element, $N_{\text{azimuth}}$, with the proportionality constant $c_{\text{azimuth}}$ [85].

$$N_{\text{azimuth}} = \left\lceil c_{\text{azimuth}} \cdot i \right\rceil,$$

(49)

A higher value for $c_{\text{azimuth}}$ corresponds to a finer discretization. The case depicted in Figure 12 corresponds to a $c_{\text{azimuth}}$ of 1. For actual calculations, a fine discretization of the polar angle might be more important than a very fine discretization of the azimuth angle. Therefore, values of $c_{\text{azimuth}} < 1$ might be of interest. If $c_{\text{azimuth}}$ is chosen smaller than one, $N_{\text{azimuth}}$ is rounded to the next larger integer. In case of $c_{\text{azimuth}} = \frac{1}{4}$ this results in one azimuth angle interval for the first four polar angle intervals, and in two azimuth angle intervals for the second four polar angle intervals.

Given a pre-defined set of angles, one has to follow a consistent convention for the ordering of these channels. In the 2D case it is an obvious choice to order all polar angle values from small to large. In 3D, a representation is chosen, where the azimuth angle channels associated to one polar angle interval are placed next to each other. Therefore, each matrix should be of the following form:
System symmetries

Another important aspect getting relevant in the 3D case is the use of system symmetries. Using such symmetries can save time in the OPTOS calculation and especially during the calculation of the redistribution matrices. For systems incorporating rotational or mirror symmetries with regard to the azimuth angle, it is not necessary to calculate the system’s response for light incoming from all angles of the chosen discretization between 0° and 360°. For example, the calculation of a redistribution matrix for an inverted pyramid surface requires only a simulation of azimuth angles between 0° and 45° since all information about other incoming angles can be determined by using the rotational and mirror symmetries of the system. While making use of the symmetry, care has to be taken that the chosen angle discretization has the same symmetry. For a 45° symmetry element, this is depicted in Figure 12 (d) for the inner four polar angle intervals up to \( i = 4 \) and \( c_{\text{visually}} \) chosen equal to 1. [85]

Absorptance inside surface textures

Mathematically, a surface is a two-dimensional object and cannot absorb any light. However, for the calculation of redistribution matrices often three dimensionally extended surface structures are considered. A pyramidal texture used for the calculation of redistribution matrices for example does not only consist of the pyramidal-shaped surface area, but of full pyramids filled with silicon. This means that the surface structure itself can absorb light, which is not directly visible in a reflection or transmission matrix. OPTOS is in principle capable of separating absorption within a surface structure from absorption within the bulk. There are different methods to do so, one being described in detail in [85]. Generally, it is important to evaluate if such a separation is necessary or if the surface structure absorption is a minor effect.

3.2.4 Basic mathematical formulation of OPTOS for 3D systems with more than two interfaces

The OPTOS formalism as presented in the previous sections is designed for the simulation of sheets with two textured interfaces. In the following, the OPTOS formalism is extended for systems with more than two interfaces, based on the third OPTOS publication [86]. Again, the fundamental principle stays the same, but additional steps are included to combine several interfaces into an effective interface in a way that in the end the OPTOS formalism as presented in the previous sections can be used. OPTOS thereby gets capable of modelling for example photovoltaic modules with additional glass or EVA encapsulation layers that could incorporate surface structures as well.
At first a naming convention specifying all different interfaces has to be introduced. This is shown in Figure 13. As before, each interface is described by four matrices: two reflection and to transmission matrices for light incident from above and below the interface, respectively.

Figure 13: Schematic view of a system with three textured interfaces. Light impinging from the top is redistributed at each interface into different transmission and reflection angles. Including the incoming light directions, “up” (blue) and “down” (orange), there are four distinct matrices which describe each interface. [86]

The basic approach to reduce such a system to a two-interface system as depicted in Figure 11 is the merging of two interfaces into one effective interface. The calculation of the effective matrices for an effective interface is done based on the light redistribution of two interfaces and propagation through the enclosed single layer. In general, any layer can be chosen for this calculation. Without loss of generality, one can look at the example depicted in Figure 14 and start with the effective reflection of the upper layer for light incident from above, \( R_{down} \) (corresponding to glass/EVA layer in the PV module case).
Figure 14: The top and the middle interface are summarized to one effective interface (on the right), which exhibits the same redistribution properties as the layer with two textured interfaces (on the left). [86]

In a similar way as in the matrix based description in section 3.2.2, the total reflection, for example, is composed of different parts. The first part is the direct reflection ($R_{3 \text{down}}$), the second has to be transmitted at the top interface ($T_{3 \text{down}}$), propagate to ($D_{\text{glass}}$) and be reflected at the middle interface ($R_{2 \text{down}}$), propagate back ($D_{\text{glass}}$) and be transmitted at the top interface ($T_{1 \text{down}}$). This is mathematically described by the matrix product $T_{3 \text{up}} D_{\text{glass}} R_{2 \text{down}} D_{\text{glass}} T_{1 \text{down}}$. The third and all further parts take additional cycles through the layer, $D_{\text{glass}} R_{2 \text{down}} D_{\text{glass}} R_{3 \text{up}}$, before the light is transmitted through the top surface. These considerations lead to the following expression for the effective interface reflection [86]:

$$R_{2 \text{eff}} = R_{3 \text{down}} + T_{3 \text{up}} \left[ \sum_{i=0}^{\infty} (D_{\text{glass}} R_{2 \text{down}} D_{\text{glass}} R_{3 \text{up}})^{i} \right] D_{\text{glass}} R_{2 \text{down}} D_{\text{glass}} T_{1 \text{down}}, \quad (51)$$

where $i$ indicates the number of cycles the light has to go downwards and upwards inside the layer. Following the same approach for light incident from below and for the transmission through the effective interface, results in the other three effective matrices [86]:

$$T_{2 \text{eff}} = T_{2 \text{down}} \left[ \sum_{i=0}^{\infty} (D_{\text{glass}} R_{3 \text{up}} D_{\text{glass}} R_{2 \text{down}})^{i} \right] D_{\text{glass}} T_{1 \text{down}}, \quad (52)$$

$$R_{2 \text{eff}} = R_{3 \text{up}} + T_{3 \text{down}} \left[ \sum_{i=0}^{\infty} (D_{\text{glass}} R_{3 \text{up}} D_{\text{glass}} R_{2 \text{down}})^{i} \right] D_{\text{glass}} R_{3 \text{up}} D_{\text{glass}} T_{2 \text{up}}, \quad (53)$$

$$T_{2 \text{eff}} = T_{3 \text{up}} \left[ \sum_{i=0}^{\infty} (D_{\text{glass}} R_{2 \text{down}} D_{\text{glass}} R_{3 \text{up}})^{i} \right] D_{\text{glass}} T_{2 \text{up}}. \quad (54)$$
Similar to the infinite sum in equation (41), the sums in the effective matrices can again be calculated iteratively with a finite \( i_{\text{max}} \) or by using the geometric series for matrices (Neumann series), which leads to the following form:

\[
R_{2,\text{eff}}^{\text{down}} = R_3^{\text{down}} + T_3^{\text{up}} \left[ I - (D_{\text{glass}} R_2^{\text{down}} D_{\text{glass}} R_3^{\text{up}}) \right]^{-1} D_{\text{glass}} R_2^{\text{down}} D_{\text{glass}} T_3^{\text{down}},
\]

\[
T_{2,\text{eff}}^{\text{down}} = T_2^{\text{down}} \left[ I - (D_{\text{glass}} R_3^{\text{up}} D_{\text{glass}} R_2^{\text{down}}) \right]^{-1} D_{\text{glass}} T_3^{\text{down}},
\]

\[
R_{2,\text{eff}}^{\text{up}} = R_3^{\text{up}} + T_3^{\text{down}} \left[ I - (D_{\text{glass}} R_2^{\text{up}} D_{\text{glass}} R_3^{\text{down}}) \right]^{-1} D_{\text{glass}} R_2^{\text{up}} D_{\text{glass}} T_3^{\text{down}}.
\]

\[
T_{2,\text{eff}}^{\text{up}} = T_2^{\text{up}} \left[ I - (D_{\text{glass}} R_3^{\text{down}} D_{\text{glass}} R_2^{\text{up}}) \right]^{-1} D_{\text{glass}} T_3^{\text{up}}.
\]

After the calculation of an effective matrix for the two top interfaces in Figure 13, the OPTOS formalism as described in the previous sections can be applied for the calculation of the optical properties of the complete system. By repeating such an effective matrix calculation, OPTOS can, in principle, handle an arbitrary number of interfaces.

### 3.2.5 Exemplary propagation and redistribution matrices for 2D, 3D and multilayer OPTOS

A key part of the OPTOS formalism is the use of matrices for the description of light propagation and redistribution. This allows for a numerically efficient calculation (as for matrix multiplication, inversion etc. well-developed algorithms are available), but also for some insight into the mechanisms of surfaces and interfaces. A graphical representation of the matrices in a two dimensional plot assigning color values to the matrix entries enables an intuitive understanding of their impact on the light paths.

**Propagation matrix**

Assuming a 2D case with an equidistant spacing of polar angle channels with respect to \( \sin(\theta) \), Figure 15 shows a propagation matrix as defined in eq. (28) for a 200 \( \mu \text{m} \) thick silicon sheet and a wavelength of 1100 nm. During propagation, no light is redistributed into other angle channels and hence the corresponding matrix has only diagonal entries. Absorption within the silicon decreases the power fraction in each angle channel according to Lambert-Beer’s law. For oblique angles the light path through a sheet with a certain thickness is longer and thus the matrix entries are smaller for higher angles.
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Figure 15: Example propagation matrix for a 200 µm thick silicon sheet at a wavelength of 1100 nm.

Redistribution matrices 2D

Assuming the same angular discretization, Figure 16 shows the reflection matrix of a planar interface from silicon to air calculated according to Fresnel’s formulas. As the reflection strongly depends on the polarization of light, all examples in this section show unpolarized matrices with polarization-averaged entries.

Figure 16: Redistribution matrix of a planar interface from silicon to air. There are only diagonal entries due to specular reflection. For angles larger than approx. 16° total internal reflection occurs and values of 1 appear in the reflection matrix. For angles below 16° polarization-averaged reflection values have been calculated according to Fresnel’s formulas.

Figure 17 shows a further example for a reflection matrix: V-grooves in silicon with an opening angle of the grooves of 70.52° related to the 111-planes in c-Si. The corresponding matrix was calculated with the ray tracing tool Raytrace3D [82]. As the reflection is not specular, the matrix shows primarily off-diagonal entries.
The 2D graphical representation offers an intuitive understanding of the interaction of light with a specific surface. A further visualization that supports such understanding is a plot of the column sums of a redistribution matrix. Figure 18 shows the column sums for the V-groove matrix. The column sums of such a reflection matrix show the complete reflection for a specific incident angle regardless into which direction the reflected light is redirected. The low values slightly above 30% for angles at around 45° for example are related to direct transmission as at these incident angles light impinges normally onto the V-groove flanks. There are also angular ranges where, due to total internal reflection, absolutely no transmission occurs. With respect to optimizing texture combinations for the front and the rear of silicon solar cells, the investigation of column sums allows for a basic understanding. Furthermore, it is a valuable way of validating newly calculated matrices, as effects related to physically unreasonable light paths can become clearly visible.

To demonstrate also an interface that has to be described wave optically, Figure 19 shows a reflection matrix for a line grating in silicon (period 990 nm, binary profile, fill factor 0.5, grating depth
160 nm). This matrix has been calculated using RCWA. Discrete orders of diffraction are clearly visible and the strength of the diagonal entries directly shows the strength of the 0\textsuperscript{th} order.

Figure 19: Redistribution matrix of a line grating interface from silicon to air. Discrete orders of diffraction (0\textsuperscript{th}, 1\textsuperscript{st}, 2\textsuperscript{nd}) are visible for normal incidence. For oblique incidence, these orders split up into -1\textsuperscript{st} and +1\textsuperscript{st} or -2\textsuperscript{nd} and +2\textsuperscript{nd}, respectively [84].

Redistribution matrices 3D

Many interfaces can only be described correctly in three dimensions. As described in section 3.2.3, an additional angle, the azimuth angle $\varphi$, has to be introduced. This complicates a simple graphical representation of redistribution matrices. However, as the change of polar angles is often the most relevant quantity, it can be an option to average a 3D matrix over all incident azimuth angles $\varphi$ corresponding to the same polar angle (meaning averaging matrix columns) and to sum all outgoing values corresponding to different $\varphi$ values but the same polar angle (meaning summing of corresponding entries within one matrix column). This procedure yields pseudo-3D matrices that can be graphically represented in the same way as in the 2D case. Figure 20 shows such a pseudo-3D reflectance matrix for an inverted pyramids surface from silicon to air. Similarly to the V-groove system, the calculation was done with the ray tracing tool Raytrace3D. As a pyramidal surface leads to similar light paths than a V-groove system but allows for even more different light paths, the matrix shows some similarity to the V-groove matrix but has much less distinct entries.
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Figure 20: Reflection matrix for a regular inverted pyramid front side at wavelength of 1100 nm calculated via ray tracing. Left: a sketch of light interaction with the silicon-air surface. Right: a simplified pseudo-3D version of the matrix where all entries of different $\phi$-values have been summarized only into the dependency of $\theta$. [85]

A further important surface texture that will be used frequently within this work is a Lambertian scattering interface. Such a surface scatters the light independently of the incident angle into all other directions with a cosine-characteristic:

$$I(\theta) \propto \cos(\theta) \, . \quad (59)$$

This means that the incident power is redistributed uniformly among the angle channels, if they have the same projected area (see Figure 12 for visualization of projected area). The discretization with equally distributed $\sin(\theta)$-values for the polar angle and the symmetry constraints for the azimuth angle (as described in section 3.2.2) results in very similar but not in exactly equally large angle channel sizes. Therefore, the analytically calculated reflection matrix as depicted in Figure 21 (b) shows an almost uniformly distributed power over the channels. In Figure 21 (b) the complete matrix is shown for all angle channels (discretized in $\varphi$ and $\theta$). In Figure 21 (c) the simplified pseudo-3D version of the matrix depending only on the polar angle $\theta$ as presented in the previous examples is shown. In this representation, large outgoing angles seem to be more pronounced. However, this results only from the fact that for large polar angles the corresponding solid angle gets larger.
Figure 21: Reflection matrix for a Lambertian scatterer calculated analytically. (a) schematically shows the interaction of light at a Lambertian surface. (b) shows the complete redistribution matrix with all polar and azimuth angles. (c) shows the simplified pseudo 3D-version.

This example with two representations of the same structure looking very differently already shows that any interpretation of such graphically represented matrices has to be done carefully and can also be misleading. Especially the underlying angle discretization strongly influences the final appearance of the matrix.

**Effective redistribution matrices for multilayer OPTOS**

As described in section 3.2.4, for the multilayer OPTOS approach two or more interfaces are summarized into one effective interface. As an example, Figure 22 shows the matrices for a typical solar module front surface: air to EVA (the glass is neglected in this example, as it has very similar optical properties to EVA) to silicon textured with random pyramids. Figure 22 (a) shows in the upper part the two-dimensional sketch of a planar EVA-air and a silicon-EVA interface textured with random pyramids. The two individual internal reflectance properties are described by the reflectance matrices, (b) and (c), respectively. The effective interface in the lower part of (a) is represented by the effective matrix in (d). Comparing matrices (c) and (d) shows larger values close to the diagonal for
the effective system. Thus, the matrix for the complete system in (d) can be understood as kind of a sum or mixture of the two individual matrices (b) and (c). The physical explanation for the larger values close to the diagonal in (d) compared to (c) is the additional specular internal reflection at the planar EVA-air interface. A large fraction of the light that is transmitted from the silicon to the EVA is reflected at the front surface and re-enters the silicon with the same angle.

Figure 22: Sketches of EVA-air, Si-EVA and effective Si-EVA-air interfaces in (a). The redistribution matrices (b) and (c) correspond to the two individual interfaces and (d) shows the effective matrix combining the two interfaces. All reflection matrices describe the internal reflection properties of light incident from below. [86]

3.2.6 Validation and comparison to existing methods and measurements
As OPTOS is a completely new development within this work (together with Nico Tucher in his dissertation [65]), a thorough validation was carried out including convergence analyses, comparison to well established simulation methods and to measurements. To quickly summarize, the results
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obtained with OPTOS (2D, 3D and multilayer) are in very good accordance to both, alternative simulation techniques for systems where such alternative techniques are available, and to measurements. All three publications dealing with the OPTOS method contain detailed validation investigations. Here, I want to present 4 exemplary validations.

**Planar front– grating at the rear**

The first system presented for validation is a silicon sheet featuring a planar front surface and different line gratings at the rear. As light in such a system propagates only within one plane (e.g. the x-z-plane), this can be solved with matrices considering only a discretization of the polar angle. Of course also 3D matrices including different φ-values can be used, but this will not change the result while significantly increasing the numerical effort. Such systems have also been investigated by Mellor et al. [87]. In his work, the systems consist of a 40 µm thick silicon sheet with a 114 nm thick SiO₂-antireflection coating on the front and a binary grating at the rear side. Between the silicon grating and an ideal dielectric reflector (refractive index \( n = 100000 \)), there is an additional dielectric buffer layer (DBL) made of SiO₂ with a thickness of 1 µm. The grating parameters are in the first case a period of 990 nm and a depth of 160 nm and in the second case a period of 350 nm and a depth of 180 nm. The volume fill factor of the grating is in both cases 0.5. The simulation results of Mellor (solid lines) and obtained with OPTOS (dashed lines with symbols) are shown in Figure 23. An additional reference with planar front and planar rear was calculated with TMM and OPTOS. For all systems the OPTOS results show an excellent agreement to the established reference methods.

![Figure 23: Calculated absorptance for a silicon wafer with a thickness of 40 µm. The black line shows the absorption of a planar reference wafer calculated by TMM. The orange triangles show the results for the same system obtained by OPTOS. The orange circles and rhombs are OPTOS calculations for systems with planar front and a line grating at the rear. Grating 1 has a period of 990 nm and a grating depth of 160 nm, grating 2 a period of 350 nm and a depth of 180 nm. The results are compared to calculations of Mellor [87], where the diffraction orders of the gratings are directly used as angle channels. [84]](image)
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A similar system has also been realized experimentally and photospectrometric measurements are compared to OPTOS results in Figure 24. In this case a 250 µm thick silicon wafer with a binary line grating (period 410 nm, grating depth 120 nm) at the rear was used. The very good agreement between measurement and simulation visible in Figure 24 further validates OPTOS.

Figure 24: Calculated and measured absorptance for a silicon wafer with a thickness of 250 µm and a binary line grating on the rear side. The measured absorption is in good accordance to the absorption calculated using OPTOS. [84]

Furthermore, for a system with planar front and a crossed grating at the rear, which requires a discretization of $\phi$ and $\theta$, convergence with respect to the angle discretization has been investigated. In this case a grating period of 990 nm, a grating depth of 160 nm and an area related fill factor of 0.25 were assumed. Since light propagates only in a finite set of diffraction orders, the absorptance can also be calculated using the formalism of Mellor et al. [54]. The Mellor method yields an exact result with regard to the angular discretization, as all directions of light propagation are well defined by the first interaction of light with the grating and can be used as angle channels. This turns the Mellor method into a perfectly suited reference method for a convergence analysis. To determine a sufficiently fine angle discretization for the OPTOS simulations, redistribution matrices with a polar angle resolution of 100 intervals have been conducted and the number of azimuth angle channels was varied. The resulting total absorptance for a system with 100 µm sheet thickness is depicted in Figure 25 for different values of $c_{\text{ azimuth}}$ as defined in eq. (49). Sufficiently small differences between the exact solution and the simulation are reached for a proportionality constant of $\frac{1}{4}$. A similar convergence analysis was carried out for the number of polar angle intervals. Based on this analysis, a number of 75 intervals was found to be sufficient and is used for all following simulations.
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Figure 25: Convergence analysis with respect to the azimuth angle $\varphi$. The total absorptance of a system with planar front and crossed grating at the rear side was calculated for different numbers of azimuth angle channels and compared with an exact discretization as used by the Mellor method. [85]

Pyramidal front–planar rear

For this second system featuring a front surface textured with pyramidal structures, the use of 3D matrices is required. An exemplary corresponding pseudo-3D matrix for regular inverted pyramids was depicted in Figure 20. However, regular pyramids are not suitable for a comparison between ray tracing and OPTOS. When calculating a redistribution matrix, homogenous illumination of an interface is assumed. But during ray tracing of a complete system with regular pyramids on one side and a planar interface on the other side, the pyramids are not illuminated homogeneously but certain facets are hit with higher probabilities depending on the sheet thickness and pyramid dimensions. This has been described in detail in [27]. Such an inhomogeneous illumination originating from a special geometrical relation of light paths with front and rear side is not considered in OPTOS (and also questionable for realistic simulations, as ray divergence and small sheet thickness deviations wash out such geometrical effects). This has to be kept in mind when comparing OPTOS simulations with full ray tracing. Comparisons of simulations with random and regular pyramids can be found in [85] and shall not be further examined here. Figure 26 shows simulations and measurements for a system with random upright pyramids at the front and a planar rear. As reference simulation method, the wafer ray tracer of PV-Lighthouse was used. The simulated wafer thickness was 200 $\mu$m with a pyramid height of 3.6 $\mu$m, and 500,000 rays were traced. As can be seen in the short wavelength range, measurement and both simulations feature the same front surface reflection and as can be seen in the long wavelength range also the light trapping properties are in good accordance. The measurement shows a slightly higher absorptance between 1050 and 1150 nm. As both simulations techniques almost perfectly match, possible reasons for this can be imperfections in the fabricated pyramids that lead to additional scattering or a beam divergence that is not accounted for in both simulations.
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Figure 26: Absorptance spectra for a 200 µm thick silicon wafer with random upright pyramids at the front and a planar surface at the rear. The black line shows a planar-planar reference.

Random upright pyramids at the front – planar rear (module configuration in EVA)

The third system for validation is a typical silicon solar module with a glass-EVA front surface, a random upright pyramid texture at the front of a 160 µm thick silicon wafer and a white backsheet with a Lambertian scattering characteristic. Thus it includes several effective interface matrices. As reference method the PV-Lighthouse module ray tracing tool was used. Figure 27 shows the absorptance in the silicon bulk determined by PVL and by OPTOS. The simulations are in very good accordance over the complete wavelength range and thus validate the multilayer OPTOS approach.

Figure 27: Absorptance and reflectance of an encapsulated thick silicon sheet with random pyramids as front side texture and a perfect planar reflector at the rear side. The simulations results of the OPTOS module formalism and PV-Lighthouse ray tracing agree very well over the whole spectral range.

In conclusion, three different systems have been investigated for the validation of OPTOS. Both, well established simulation techniques and optical measurements have been used for comparison and
3 Methods for the optical simulation of light trapping in solar cells

overall, very good agreement was found and OPTOS can be used for investigation, optimization and comparison of light trapping structures. In chapters 5 and 6, manifold simulation results based on OPTOS will be presented.
4 Simulation and experimental realization of antireflection systems

Good front side antireflection systems are necessary to reach high currents in solar cells. With regard to a possible combination of antireflection systems at the front with additional light trapping structures at the rear, in this chapter wave optical simulation techniques are applied to optimize multilayer planar antireflection coatings and to investigate black silicon, respectively. Both these concepts are promising alternatives to the standard pyramidal front side textures. This chapter is based on results of the master project of Alexander Bett, which I supervised [90].

4.1 Multilayer planar antireflection coatings

The use of planar antireflection coatings is a standard method for many optical components to suppress surface reflections between two media with differing refractive index. As described in the introduction, the use of a standard SiN₆-antireflection coating on a silicon solar cell reduces the averaged surface reflectivity from 35% to 9%. In this section, I present a systematic, simulation based analysis, how the reflectivity can be further suppressed by the use of multilayer planar antireflection coatings. The results within this section have been developed together with Alexander Bett within his master thesis [90], where also a detailed description of the methods and results can be found. As the relevant steps in the refractive index step are different for a solar cell (air to silicon) and a solar module (air to glass/EVA to silicon), all investigations have been conducted for both, solar cells and complete solar modules with encapsulation.

Figure 28: The two investigated systems, planar multilayer antireflection coatings in a module and on a solar cell (simplified system).
4.1.1 Optimization parameters

For an efficient solar cell the quantity that has to be maximized is the amount of light \( T \) that is transmitted into the electrically active silicon bulk material. It is crucial to maximize \( T \) instead of minimizing the reflectivity \( r \), because there is a further loss mechanism: the parasitic absorption in the antireflection coating. To obtain a quantity relevant for a highly efficient silicon solar cells, the wavelength dependent transmission has to be weighted with the AM1.5g spectrum and with an IQE of a highly efficient silicon solar cell. This weighted transmission \( T_{w,\text{cell}} \), which is the final optimization parameter for solar cells, is then given by

\[
T_{w,\text{cell}} = \frac{\int_{280}^{1200} T_{\text{air-si}}(\lambda) \cdot N_{\text{AM1.5g}}(\lambda) \cdot \text{IQE}(\lambda) d\lambda}{\int_{280}^{1200} N_{\text{AM1.5g}}(\lambda) \cdot \text{IQE}(\lambda) d\lambda}.
\] (60)

Note, that \( T_{w,\text{cell}} \) is not an actual transmittance that could be measured with a spectrometer, as it is based on a wavelength dependent weighting. It is just a fitness parameter that allows for comparing different systems with regard to the amount of light that is transmitted into the silicon bulk. For a complete module an additional interface from air to glass/EVA and parasitic absorption within the glass/EVA has to be considered and the antireflection coating has to be optimized for the refractive index step from glass/EVA to silicon. To account for the first, an additional weighting function containing the transmission through the glass/EVA interface has to be added and to account for the latter, the transmission from EVA to silicon has to be considered instead of air to silicon:

\[
T_{w,\text{module}} = \frac{\int_{280}^{1200} T_{\text{EVA-si}}(\lambda) \cdot N_{\text{AM1.5g}}(\lambda) \cdot \text{IQE}(\lambda) \cdot T_{\text{Glass/Eva}}(\lambda) d\lambda}{\int_{280}^{1200} N_{\text{AM1.5g}}(\lambda) \cdot \text{IQE}(\lambda) \cdot T_{\text{Glass/Eva}}(\lambda) d\lambda},
\] (61)

Again, also \( T_{w,\text{module}} \) is a fitness parameter and not an actual transmittance due to the weighting and must not be confused with \( 1-r \), for example. Figure 29 shows the three weighting functions of the equations (60) and (61). The transmittance \( T_{\text{Glass/Eva}}(\lambda) \) has been calculated using RAT [68] with layer thicknesses typical for a module (3 mm glass, 460 \( \mu \)m EVA). As depicted in Figure 29 it reduces the complete transmission function by a factor of approximately 0.96 for all wavelengths due to the air-glass reflection and significantly reduces the influence in the UV as EVA strongly absorbs light below 400 nm.
Simulation and experimental realization of antireflection systems

Figure 29: Weighting functions for the calculation of the weighted transmission into the active silicon bulk. For solar cells only the AM1.5g spectrum and the IQE are used, for modules additionally the transmission through glass and EVA has to be considered.

For the comparison of measurements and other simulation results, where the fitness parameters defined in equations (60) and (61) are not easily accessible, the weighted reflectance can be used. When typical silicon wafers with thicknesses of 200 µm are used, the reflectance for wavelengths larger than 1000 nm contains internal rear reflections in addition to the front surface reflectivity. As the focus of this chapter is the reduction of front surface reflectivity, the reflectance values are therefore averaged and weighted with the AM1.5g spectrum just between 280 and 1000 nm:

\[
\begin{align*}
    r_w = \frac{\sum_{\lambda=280}^{1000} N_{AM1.5g}(\lambda) \cdot R(\lambda)}{\sum_{\lambda=280}^{1000} N_{AM1.5g}(\lambda)},
\end{align*}
\]

(62)

4.1.2 Available materials for antireflection coatings

Figure 30 shows a large set of refractive index data, which serves as input for the optimization. All these materials have been deposited at Fraunhofer ISE and are in principle available for the use in silicon solar cells. The refractive index data have been determined with spectral ellipsometry. As the spectral ellipsometer lamp covers only the range between 250 and 990 nm, both, \( n \) and \( k \) have been extrapolated to 1200 nm. As there are no absorption peaks within the extrapolated wavelength range, such an extrapolation is not expected to introduce a significant error. Note that this data partly deviates from typical literature data, but the goal within this work was to identify the most promising materials that are actually available. In addition to the real refractive index data, also idealized data (constant, arbitrary \( n \) values and \( k = 0 \)) have been used for optimization calculations.
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4.1.3 Optimization algorithm for multilayer planar antireflection coatings

As the parameter space for a complete optimization including all the materials in Figure 30 and arbitrary layer thicknesses is very large, especially for multilayer systems, a genetic algorithm was used to find optimum material combinations and layer thicknesses. The basic working principle of this genetic approach is sketched in Figure 31. The actual optical calculation only comprises the equations (60) and (61) using TMM for the calculation of \( T_{\text{air-Si}}(\lambda) \) and \( T_{\text{EVA-Si}}(\lambda) \), respectively.

Figure 30: Real part \( n \) and imaginary part \( k \) of dielectric materials available at Fraunhofer ISE considered in the optimization of planar multilayer antireflection coatings. [90]
4.1.4 Results

4.1.4.1 Optimization of planar multilayer antireflection coatings for solar cells

Table 1 shows the results of the optimization of planar multilayer antireflection coatings for crystalline silicon solar cells. The upper case with freely chosen wavelength-independent refractive index data can be seen as kind of an upper benchmark for real materials. However, it is not an upper limit as the refractive index was assumed to be constant over the whole spectral range, while a wavelength dependent refractive index could match the condition $n_{ARC} = \sqrt{n_1 n_2}$ (for single layer ARC, more complicated relations for more layers) at each individual wavelength and thus lead to even higher weighted transmission values. The following results have to be emphasized: For a single layer ARC, there is a material (SiNxOy) with a refractive index very close to the idealized case enabling transmission values of approx. 91%. This material is also close to the standard SiNx layers frequently used in silicon solar cells. A double layer ARC with real materials (SiO2 and TiO2) can further enhance the transmission to 96%, which is 1% less than in the idealized case. This is due to the fact that there is no lossless material with a refractive index as high as 2.62, which would be required in the idealized case. For the three layer ARC this restriction gets even more important and for real materials the transmission can only be enhanced by 0.3%. In the idealized case, lossless materials with high refractive indices above 3 allow for a further significant increase of the transmission, but this is a very hypothetical case as such materials are not available as dispersion and high real parts of the refractive index are always correlated with absorption. Already this result shows that a two layer system might be the practical optimum. A third layer does not significantly increase the transmission but increases the complexity of involved processes. Note that this is a purely optical optimization and other
demands like passivation properties or etching behavior that may also be important for a solar cell are not included here.

Table 1: Optimization results of planar antireflection coatings for silicon solar cells. The top part contains results for freely selectable \( n \) values and \( k = 0 \). The middle part contains actually available materials. All given refractive indices refer to a wavelength of 650 nm. The bottom part contains measured thicknesses and reflectivity values of systems fabricated based on the optimization in the middle part.

<table>
<thead>
<tr>
<th>Simulation with idealized ( nk )-data</th>
<th>3 layer ARC</th>
<th>2 layer ARC</th>
<th>1 layer ARC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Superstrate</td>
<td>Air</td>
<td>Air</td>
<td>Air</td>
</tr>
<tr>
<td>Optimized thicknesses</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Optimized thicknesses</td>
<td>109.8 nm</td>
<td>n = 1.31</td>
<td>103.3 nm</td>
</tr>
<tr>
<td>Optimized thicknesses</td>
<td>72.0 nm</td>
<td>n = 2.04</td>
<td>54.1 nm</td>
</tr>
<tr>
<td>Optimized thicknesses</td>
<td>41.7 nm</td>
<td>n = 3.12</td>
<td></td>
</tr>
<tr>
<td>Substrate</td>
<td>Silicon</td>
<td>Silicon</td>
<td>Silicon</td>
</tr>
<tr>
<td>Fitness parameter ( T_w )</td>
<td>98.9%</td>
<td>97.3%</td>
<td>91.1%</td>
</tr>
<tr>
<td>Weighted reflectivity ( r_w )</td>
<td>1.6%</td>
<td>3.5%</td>
<td>10.3%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Simulation with real ( nk )-data</th>
<th>3 layer ARC</th>
<th>2 layer ARC</th>
<th>1 layer ARC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Superstrate</td>
<td>Air</td>
<td>Air</td>
<td>Air</td>
</tr>
<tr>
<td>Optimized thicknesses</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Optimized thicknesses</td>
<td>94.1 nm</td>
<td>MgF(_2) 1.38</td>
<td>96.7 nm</td>
</tr>
<tr>
<td>Optimized thicknesses</td>
<td>29.2 nm</td>
<td>Si(_N), (_O) 1.94</td>
<td>59.3 nm</td>
</tr>
<tr>
<td>Optimized thicknesses</td>
<td>47.0 nm</td>
<td>TiO(_2) 2.32</td>
<td></td>
</tr>
<tr>
<td>Substrate</td>
<td>Silicon</td>
<td>Silicon</td>
<td>Silicon</td>
</tr>
<tr>
<td>Fitness parameter ( T_w )</td>
<td>96.4%</td>
<td>96.1%</td>
<td>90.7%</td>
</tr>
<tr>
<td>Weighted reflectivity ( r_w )</td>
<td>3.3%</td>
<td>3.6%</td>
<td>8.7%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Measurement</th>
<th>3 layer ARC</th>
<th>2 layer ARC</th>
<th>1 layer ARC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Superstrate</td>
<td>Air</td>
<td>Air</td>
<td>Air</td>
</tr>
<tr>
<td>Fabricated thicknesses</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fabricated thicknesses</td>
<td>101 nm</td>
<td>MgF(_2) 1.38</td>
<td>103 nm</td>
</tr>
<tr>
<td>Fabricated thicknesses</td>
<td>37 nm</td>
<td>Si(_N), (_O) 1.94</td>
<td>62 nm</td>
</tr>
<tr>
<td>Fabricated thicknesses</td>
<td>44 nm</td>
<td>TiO(_2) 2.32</td>
<td></td>
</tr>
<tr>
<td>Substrate</td>
<td>Silicon</td>
<td>Silicon</td>
<td>Silicon</td>
</tr>
<tr>
<td>Weighted reflectivity ( r_w )</td>
<td>3.5%</td>
<td>3.7%</td>
<td>10.0%</td>
</tr>
</tbody>
</table>

The optimized systems have been fabricated and characterized using spectral ellipsometry and spectrophotometry. TiO\(_2\) and MgF\(_2\) have been evaporated, Si\(_N\), \(_O\) and SiO\(_2\) deposited via PECVD.
The resulting thicknesses and reflectivity values are also listed in Table 1. For both techniques a deviation from the layer thickness to the desired value of 5 to 10 nm occurs. Figure 32 shows the spectrophotometric characterization of the three systems in comparison to simulations of the optimized systems. Obviously, a single layer ARC is much more sensitive to deviations in the layer thickness. As it features one distinct reflection minimum, a change in the layer thickness directly causes a shift of the spectral position of this reflection minimum. Two and three layer ARCs are more robust to such deviations due to their spectrally broader reflection minima, which could be an advantage in terms of processing. The fabricated ARC containing three layers - like the simulated one - shows only a very small further reduction of the reflectivity. Hence, the two layer system proves to be the most reasonable compromise between low reflectivity and high process complexity. Figure 32 shows also SEM cross sections of the three fabricated systems.

Figure 32: Comparison of measured and simulated reflectance, transmittance and absorptance for single, double and triple layer ARC. The deviations mainly originate from differences in the layer thicknesses. The SEM pictures show cross sections of the fabricated systems. Based on [90].

In order to quantitatively compare the optimized results to a standard front surface with a pyramidal texture, also wafers within this investigation have been textured with inverted pyramids and a single layer ARC (64 nm SiNx) has been deposited resulting in an averaged reflectivity of 3.1 %. This is slightly below the reflectivity of a two or three layer planar ARC and can be further reduced as the fabricated pyramids featured ridge tops with a width of up to 1 µm (base width of the pyramids
20 μm) leading to planar areas. The simulation of random upright pyramids, which allow for even lower surface reflectivities as they feature no planar ridge tops, results in an averaged reflectance of 1.8%.

Summarizing, planar multilayer systems have been optimized and fabricated for solar cells with averaged reflectivities down to 3.5%. This is still slightly higher than values that are reached with the standard front side, pyramidal textures and a single layer ARC, that allow for values below 2%. However, a planar front surface might feature other advantages and this optimization provides an alternative option featuring only slightly higher front side reflectivities than the state-of-the-art technique.

**4.1.4.2 Optimization of planar multilayer antireflection coatings for solar modules**

The same optimization as described above has been conducted for a complete module structure (as depicted in Figure 28) including glass and EVA and also a dielectric passivation layer between ARC layers and the silicon bulk. Table 2 summarizes the results. The refractive index of EVA (approx. 1.5) prevents low refractive index materials like MgF₂ or SiO₂ to be chosen within the genetic algorithm. This makes it even more difficult to find suitable materials for a multilayer ARC. On the other hand, the fact that EVA absorbs most of the UV light enables the use of materials with a higher absorption coefficient in the UV. Therefore, in this module optimization partly different materials compared to the cell optimization appear. This result strongly emphasizes the need to investigate the optical properties of front textures and materials not only on solar cell level, but on the final module level. This, however, comes for the prize, that a solar cell optimized for the use in a module will perform worse when the cell itself is measured under STC.

Table 2: Optimization results of planar antireflection coatings for silicon solar modules with EVA and glass cover. All given refractive indices refer to a wavelength of 650 nm.

<table>
<thead>
<tr>
<th>Simulation with real nk-data</th>
<th>3 layer ARC</th>
<th>2 layer ARC</th>
<th>1 layer ARC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Superstrate Air Air Air</td>
<td>Module Air Glass 3 mm Glass 3 mm Glass</td>
<td>460 µm EVA 460 µm EVA 460 µm EVA</td>
<td>460 µm EVA 460 µm EVA 460 µm EVA</td>
</tr>
<tr>
<td>Optimized thicknesses 70.5 nm SiNₓOᵧ 1.80</td>
<td>68.9 nm SiNₓOᵧ 1.80</td>
<td>52.0 nm TiO₂ 2.32</td>
<td></td>
</tr>
<tr>
<td>Optimized thicknesses 26.5 nm TiO₂ 2.32</td>
<td>57.7 nm TiO₂ 2.32</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Optimized thicknesses 21.5 nm SiCₓ 2.66</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Passivation 10 nm Al₂O₃ 10 nm Al₂O₃ 10 nm Al₂O₃</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Substrate Silicon Silicon Silicon</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fitness parameter T_w 96.5 % 96.0 % 94.5 %</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Weighted reflectivity r_w 7.0% 8.4% 8.9%</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
In the module case, the difference between single and multilayer coatings is significantly smaller than on solar cell level. The gain that can be reached by depositing a double or triple layer ARC instead of a single layer ARC is considerably smaller than for the solar cell itself. Overall, the reflectance losses at the solar cell front get less important when embedded in a module. Of course, an additional reflection at the front air to glass interface of approximately 4 % occurs contributing about 50 % of the total reflectance, which can also be minimized by an ARC on the glass. This was not investigated within this work as I want to focus on the solar cell itself. Again, the comparison to the most commonly used module front side, random pyramids with single layer ARC and EVA and glass cover, is an important benchmark. Using the PV Lighthouse module ray tracer [80] results in a front surface reflectance of approximately 4.7 %, which is again below the optimized planar systems. Thus, the investigated planar multilayer ARCs might be an interesting option, if a standard front side texture for other than purely optical reasons is not feasible.

4.2 Black silicon

An alternative structure for the front of silicon solar cells, which also allows for a very effective reduction of reflectance, is so called black silicon. Black silicon might have the potential to reach reflectance values even below the pyramidal standard textures and it might also feature promising properties with regard to light trapping when combined with diffractive structures at the rear. Therefore, within this work, together with Alexander Bett who investigated black silicon within his master thesis [90], I investigated the optical properties of black silicon particularly with regard to its light trapping properties. The following description is based on the results published in [91]. In general, the term “black silicon” term describes a nanostructured, stochastic surface with very low reflectance over a wide range of the solar spectrum [30,92–96], thus making it look black. The height of the structure is typically in the range of only a few hundred nanometers to a few micrometers. There are different manufacturing methods available for black silicon leading to various structure geometries and optical properties [30,92–94,97–100]. Within this work, black silicon has been fabricated by inductively coupled plasma reactive ion etching (ICP-RIE) [94] by a project partner (University Aalto, Finland). A scanning electron microscope (SEM) picture of the structure is shown in Figure 33 (a) and Figure 33 (b) shows the corresponding measured reflectance. Even without an antireflection coating, the reflectance in the range of 280 nm to 1000 nm weighted by the AM1.5g photon flux spectrum is only 1.2 %, which is significantly lower than the values presented above for planar multilayer ARCs and also lower than the values reached with standard pyramidal textures, that are between 1.5 and 2 % [28]. This highlights the excellent antireflection effect of black silicon. For the application of black silicon in solar cells, however, besides its optical properties, it is also important that the large surface can be electrically passivated. This has been achieved in the recent years using aluminum oxide deposited by atomic layer deposition [92,94,97,101].
Simulation and experimental realization of antireflection systems

Figure 33: (a) Scanning electron microscope (SEM) picture of black silicon fabricated by inductively coupled plasma reactive ion etching as considered in this work. (b) Measured reflectance of a 250 µm thick silicon wafer with black silicon at the front and a planar rear. The reflectance in the range of 280 nm to 1000 nm weighted by AM1.5g is 1.2%. [91]

Within this work, the optical properties of black silicon, especially the angular characteristic of the transmitted light have been investigated with optical measurements and wave optical simulations. The angular characteristic of the light transmitted through a black silicon surface into the silicon bulk is of great interest, especially for the combination with additional light trapping structures at the rear. Before the detailed wave optical simulations of black silicon are presented, the question has to be answered, if black silicon could be described as a gradient index layer.

4.2.1 Black silicon as graded index layer?

Based on SEM pictures a linear relationship between depth and refractive index was used as input for TMM simulations of a gradient index layer. The continuously increasing refractive index was approximated by 1000 individual layers, each 1 nm thick. Figure 34 shows a strong deviation in the NIR between such a graded index layer simulation and the measurement. While the low reflectance of the graded index layer matches the low measured reflectance in the short wavelength range, the measured absorptance in the NIR is significantly higher than the one simulated based on a graded index layer. As a graded index layer does not lead to any change of direction for normally incident light, this indicates that the light in the measured sample is in some way redirected, leading to longer light paths and thus higher absorptance. Note that this investigation as all following investigations have been done with one example black silicon structure with specific feature sizes. For other black silicon samples featuring different characteristic sizes or geometries, the results are not valid and the investigations would have to be repeated.
Simulation and experimental realization of antireflection systems

Figure 34: Description of black silicon as graded index layer. A linear relationship between depth and refractive index based on SEM pictures has been assumed. The comparison with the measurement shows that the low reflectance in the short wavelength range is matched. However, the absorptance in the NIR, which is related to the scattering properties, strongly deviates. Based on [90].

4.2.2 Scattering properties of black silicon determined by RCWA

As indicated in the section before, black silicon leads to a redirection of light within the silicon bulk. To investigate the detailed scattering characteristics, Kroll et al. presented a formalism combining the Fourier Modal Method and an incoherent propagation method to calculate the absorptance of a wafer with a black silicon front texture [92]. They also determined the angular distribution within the silicon bulk. To build the model, they measured the surface topography by taking cross section SEM micrographs between a series of milling steps using a focused ion beam. The angular distribution was then calculated using finite difference time domain [102]. Here, I present an alternative method for simulating the optical properties of black silicon, especially the angular distribution of light within the silicon bulk after passing through the black silicon front surface. The approach is based on approximating black silicon with a simple random cone structure and using the rigorous coupled wave analysis (RCWA) for the calculation of the optical properties. The simplified cone topography allows for a more direct understanding of what creates the functionality of the black silicon and would also allow for a more targeted approach in future structure optimizations, for example by directly investigating the influence of feature height, density of “needles” (cones) etc.
As the RCWA is designed for the simulation of periodic structures, the stochastic structure of black silicon must be converted into a periodic structure. This can be done using a super cell approach: a unit cell covering an area of the black silicon surface containing stochastically varying needle structures is repeated periodically. If the super cell size is large enough, the results do not change significantly with the artificially introduced periodicity. Of course, this artificial periodicity restricts the light propagation to a set of diffraction modes defined only by the periodicity according to equation (8) making a large super cell necessary. For all occurring effects, it has to be carefully evaluated if they are originating from the black silicon structure itself or from the artificial periodicity.

4.2.2.1 Structure implementation of black silicon into RCWA

To keep the structure as simple as possible, the needle like black silicon structure was approximated by cones. The height of the cone and the diameter at the base are assigned randomly in intervals defined by results of SEM-measurements, such that all heights between 0.6 µm and 1 µm and base diameters between 0.2 µm and 0.4 µm, respectively, occur with the same probability. These values were extracted from scanning electron microscope (SEM) pictures (Figure 35). In addition, each cone is allocated to a random position \((x\text{ and } y)\) in the unit cell. The SEM pictures also show a density of needles slightly above 20 needles in an area of 1 µm². No significant planar areas can be seen in the SEM pictures. In order to match the measured needle density, while avoiding planar areas, the structure generation starts with a cone density between 19 and 20 cones per µm². For all planar areas with a diameter greater than 0.2 µm (resulting from the first randomized positioning of cones), an additional cone is added. Thus, in the end, the structure has between 20 and 23 cones per µm², which corresponds to the value determined by the SEM pictures. If a cone overlaps the edge of the unit cell, the overlapping part is shifted to the opposite side, so that there are no discontinuities in the structure when repeating the unit cell periodically. Figure 35 shows the SEM pictures, which the cone parameters are based on, and an example of a generated randomized cone structure. [91]
4.2.2.2 Reflectance, transmittance and absorptance results

Reflectance, transmittance and absorptance were determined for unit cell sizes between 1.35 µm and 2.01 µm corresponding to a number of propagating modes between 69 and 161, e.g. pairs of mode numbers \((p,q)\) at a wavelength of 1.0 µm. Since, in reality, black Si is not a periodic structure, the unit cell size used in the simulation should be as large as possible. However, the size of the unit cell is limited due to high computational demands (time and storage) for large periods. Therefore, the simulations are limited to the wavelength range between 1.0 µm and 1.1 µm, where light trapping effects are clearly visible but parasitic absorption is not yet as important as for even longer wavelengths. Figure 36 shows reflectance, transmittance and absorptance of simulated structures for two different unit cell sizes. For the smaller cell with an edge length of 1.40 µm 15 random structures were generated as described in section 3.4.2.1. For each structure, reflectance, transmittance and absorptance were calculated. The graph shows the mean value of these 15 structures. The standard
deviation is represented by error bars. For the larger unit cell with an edge length of 2.01 µm, 10 random structures were considered. For comparison, the Yablonovitch limit (eq. (18)), i.e., the absorbance of a silicon wafer with a perfect antireflection coating at the front and a Lambertian scatterer at its rear, was analytically calculated. In addition, the absorbance of a silicon wafer with a graded index layer at its front is shown. [91]

![Figure 36](image)

Figure 36: (a) The simulated reflectance and transmittance of a 250 µm thick silicon wafer with black silicon at the front agrees well with the measured data. (b) Simulated and measured absorbance compared to the absorbance of a graded index layer and an ideal diffuse scatterer (Yablonovitch limit). [91]

The simulated spectra shown in Figure 36 are in good accordance to the measurements for both unit cell sizes. This is, however, not necessarily the case for all unit cell sizes. A detailed investigation of the influence of the unit cell size to the results of reflectance and transmittance results is presented in Appendix A.

### 4.2.2.3 Angular distribution

In the previous section, RCWA simulations of the total reflectance and transmittance were presented. The following section explicitly deals with the angular distribution of the light transmitted through the modelled black silicon surface within the silicon bulk. Figure 37 shows this angular distribution for a wavelength of 1.04 µm for unit cell sizes of 1.4 µm and 2.01 µm (same unit cell sizes as presented before in Figure 36). The graph shows the percentage of the total transmittance through the cone structure in the silicon bulk in dependence of the polar angle. Due to the periodic structure, only discrete modes can propagate. The corresponding polar angles are given by the grating equation (10). As we are interested in the deviation of normally incident light from the vertical direction, the irradiance is summed over all azimuth angles for each polar angle. The larger the unit cell, the more modes can propagate and thus the more polar angles are possible. The two angular distributions presented in Figure 37 show that different angular distributions can lead to similar reflectance, transmittance and absorbance curves (see Figure 36). [91]
To determine the angular distribution in the silicon bulk after passage through a black silicon front with higher accuracy, three different unit cell sizes with edge lengths larger than 2 µm were considered (2.01 µm, 2.20 µm and 2.40 µm, corresponding to 161, 193 and 233 propagating modes at a wavelength of 1.0 µm, respectively). For such large unit cell sizes, a calculation of a complete spectrum was not possible due to restrictions of calculation time and storage. According to the unit cell analysis presented in appendix A, undesirable effects directly related to a too small unit cell can be neglected for these periods. For each unit cell size, 20 random structures were created and for each structure the angular distribution in the silicon bulk was computed at wavelengths of 0.9 µm, 1.0 µm, 1.1 µm and 1.2 µm and the results then averaged for each unit cell size separately. Since the discrete polar angles are at different positions for the different unit cell sizes, a binning is necessary when averaging over the three angular distributions. Angular intervals with a width of 5° were chosen. The fraction of transmittance values was summed up in every interval for each unit cell size. Afterwards, the binned distributions of the three unit cell sizes were averaged. Figure 38 presents the results in comparison to the angular distribution of a Lambertian scatterer. To get comparable values, the cosine distributed intensity of the Lambertian scatterer has to be integrated over the solid angle associated with the appropriate polar angle interval. If \( \theta \) is the polar angle and \( \phi \) the azimuth angle, the proportion of the total intensity \( I \) in a polar angle interval \([\theta_1, \theta_2]\) is given by [91]

\[
I = \frac{\int_{\theta_1}^{\theta_2} \int_{\phi}^{\phi} \cos \theta \cdot \sin \theta \, d\theta \, d\phi}{\int_{\theta_1}^{\theta_2} \int_{\phi}^{\phi} \cos \theta \cdot \sin \theta \, d\theta \, d\phi}.
\] (63)
Simulation and experimental realization of antireflection systems

Figure 38: Simulated angular distribution of light in the silicon bulk after passage through a black silicon structure for different wavelengths compared to the distribution of a Lambertian scatterer. Three different unit cell sizes were considered, each with 20 random structures. [91]

The angular distributions qualitatively confirm the results of the simulated absorptance shown in Figure 36. During transmission through the black silicon, light is redistributed to different polar angles. However, for high angles the fraction of transmitted light is lower than in the case of a Lambertian scatterer. Thus, the scattering effects due to black silicon are not as distinct as they would be in the case of a Lambertian scatterer. With increasing wavelength the proportion of light that is directly transmitted (polar angle $0^\circ$) increases. This is due to the fact that for larger wavelengths the ratio between wavelength and structure size increases and the structure behaves more and more like a graded index layer without scattering effects. The critical polar angle separating the escape cone of total internal reflection from the solid angle where total internal reflection occurs at the rear is between $16.2^\circ$ and $16.4^\circ$ for the wavelength range considered. Depending on the wavelength, between 25% and 35% of the light is directed into the escape cone. These values are comparable to the results of Kroll et al., who investigated two different black silicon structures with 20% to 40% of the light in the loss cone [102]. Summarizing, these RCWA calculations of a black silicon super cell allow for an understanding of the light paths below a black silicon surface, which is especially important when combining such a front texture with an additional rear structure for a further improvement of the light trapping. Such combinations of front and rear textures are investigated in the following sections.
5 Experimental realization of light trapping structures

Within this chapter I present different light trapping structures for the rear of silicon solar cells that have been developed and integrated into fully processed solar cells within this work. The first section deals with simple diffuse rear reflectors as benchmark for the more complex, diffractive structures. These investigations have been conducted together with Florian Pfeffer within his Bachelor thesis [103] that I supervised. In the second section, binary gratings and their successful integration into solar cells are presented, a work done in close cooperation with Nico Tucher [65]. The third section describes sphere gratings and also demonstrates their successful application to high-efficiency silicon solar cells. The sphere grating processes and the cell integration was partly developed together with Benjamin G. Lee during his year as guest scientist at Fraunhofer ISE.

5.1 Simple diffuse rear reflectors

Most industrially processed solar cells feature a pyramidal textured front surface and a more or less planar specular mirror at the rear. Many of the concepts investigated within this work aim to improve the light trapping by introducing additional structures at the rear and thus further enhancing the optical light path length. Any novel structure should be benchmarked against a planar, specular rear, because this is typically used in industrial standard solar cells (with some remaining surface roughness) or in high-efficiency silicon solar cells. This section presents a further benchmark structure: simple diffuse rear reflectors like typical back sheets, white paint or binder-free TiO₂ nanoparticle layers. Such simple diffuse rear reflectors external to the solar cell are also a reasonable benchmark as they can be easily applied to bifacial silicon solar cells that are produced by many manufacturers, even for monofacial modules. Various simple diffuse rear reflectors were systematically analyzed by optical and electrical measurements. White paint, TiO₂ nanoparticles, white backsheets and a silver mirror were applied to bifacial silicon solar cells and the EQE enhancement was measured for three different solar cell geometries: planar front and rear (pp), textured front and planar rear (tp), and textured front and rear (tt). The following results were obtained together with Florian Pfeffer in his Bachelor thesis [103] and the following description is based on a joint journal publication [104].
5.1.1 Diffuse rear reflectors for silicon solar cells – background

As described already in sections 2.4.3 and 2.4.4, diffuse rear reflectors have been investigated and proposed for silicon solar cells for decades with original works by Goetzberger [37] and Yablonovitch [38]. Several devices aiming for such concepts have been realized using rather simple fabrication techniques. For example, Cotter et al. [105] investigated the optical intensity of light in silicon sheets with diffuse rear reflectors and deduced, that a high refractive index of the diffuse reflector is beneficial. Berger et al. [106] applied commercial white paint as a diffuse rear reflector to 1-2 µm thin-film polycrystalline silicon solar cells and measured a short circuit current density gain of up to 2.87 mA/cm², which led to an overall $J_{SC}$ of 9.91 mA/cm². Barugkin et al. [107] used silver nanoparticles covered with a BaSO₄-based white paint as a rear reflector and used a 260 µm thick solar cell with a front textured by reactive ion etching. They reached a $J_{SC}$ of 5.7 mA/cm² between 990 and 1200 nm corresponding to a $\Delta J_{SC}$ of 2.3 mA/cm² compared to solar cells with planar front and rear. Binders used in usual white paints are organic materials with a low refractive index (1.4-1.7), which absorb light in the near infrared [108]. Therefore, a binder-free, fully covered rough rear surface with a high refractive index is advantageous. Lee et al. [109] dispersed TiO₂ nanoparticles in deionized water with a pH value of 10 and deposited them via drop coating in order to fully cover the rear with TiO₂ nanoparticles. However, the alkalized suspension can harm the rear of the solar cell. The TiO₂ nanoparticles were placed behind 2.5 µm thick crystalline silicon solar cells. They presented a $\Delta J_{SC}$ of 3.91 mA/cm² leading to an overall $J_{SC}$ of 13.46 mA/cm². In comparison, Basch et al. [108] dispersed the TiO₂ nanoparticles in pH neutral water and also compared the TiO₂ nanoparticles with white paint showing an enhanced reflectivity [108]. The TiO₂ nanoparticles were placed behind 2 µm thick amorphous silicon cells. They presented a $\Delta J_{SC}$ of 4.8 mA/cm², which leads to an overall $J_{SC}$ of 18.7 mA/cm². Ingenito et al. applied TiO₂ based white paint as rear reflectors for 180 µm thick, both side textured crystalline silicon solar cells and demonstrated a $\Delta J_{SC}$ of 0.6 mA/cm² compared to no rear reflector [110]. Frank et al. simulated the potential photocurrent density $J_{ph}$ based on the measured properties of different diffuse rear reflectors for 200 µm thick silicon wafers with three different combinations of surface morphologies: planar front and rear surface (pp), textured front (random pyramids) and planar rear surface (tp), or both sides textured with random pyramids (tt) [111]. They compared white paint, polytetrafluoroethylene (PTFE), white paper and a silver mirror. One conclusion of the work of Frank et al. was the prediction that both-side textured solar cells with a good rear reflector lead to the overall highest photo current density of the investigated structures. [104]

5.1.2 Optical characterization of diffuse rear reflectors

Table 3 lists the investigated rear reflectors and gives a short description including the processes used for applying the rear reflectors to optical samples or solar cells.
### Table 3: Investigated simple rear reflectors. Based on [104].

<table>
<thead>
<tr>
<th>Reflector Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air + Mirror</td>
<td>A silver mirror (Company: Thorlabs, reflectivity over 95% between 600 and 1400 nm) was placed behind the wafer, while a gap of air remains between the wafer and the mirror.</td>
</tr>
<tr>
<td>Air + Black Cardboard</td>
<td>Black cardboard (reflectivity lower than 3%, transmission lower than 0.4% between 600 and 1400 nm) was placed behind the wafer, while a gap of air remains between the wafer and the black cardboard.</td>
</tr>
<tr>
<td>Air + Backsheet</td>
<td>Three different white backsheets (Company: Isovoltaic, Material: 3554 and 2442w; Company: Dunmore, Material: PPE+) were located behind the wafer, while an air gap remains between the wafer and the backsheets.</td>
</tr>
<tr>
<td>White Paint</td>
<td>White paint was placed directly on the samples. (Company: OBI, Material: Premium white color; Company: Schöner Wohnen, Material: Polar white color; Company: Schmincke, Material: Acryl color, titanium white). For dense, pin-hole free coverage, three layers of white paint where applied on the wafer with a bristle brush. The single layers were dried for 2 hours at room temperature.</td>
</tr>
<tr>
<td>TiO(_2) Nanoparticles</td>
<td>TiO(_2) nanoparticles (Company: Treibacher Industrie AG, Material: TiO(_2) -100, L32090) with an average size of 1.106 µm were placed directly on the rear surface of the samples. For the TiO(_2) coating a combination of the methods established by Basch et al. [108] and Lee et al. [109] was used. 10 g rutile TiO(_2) nanoparticles were dispersed in 100 g purified water and the resulting suspension sonicated for 30 min. The silicon wafers were put onto a hot plate at a temperature of 60 °C where several drops of the suspension were applied onto the wafer for a fully covered rear surface. The coating process was repeated 5 times, with several minutes of drying in between.</td>
</tr>
</tbody>
</table>

### Basic optical characterization of rear reflectors

First, all reflectors have been compared by measuring the total reflectance in air using a spectrophotometer and an integrating sphere (Figure 39). Overall, the TiO\(_2\) nanoparticles and the mirror show the highest reflectance, but while the mirror specularly reflects all light, the nanoparticles lead to strong scattering. Acryl color and the backsheet 3554 showed the highest reflectance of the white paints and of the different backsheets, respectively. Accordingly, these materials, denoted in the following as backsheet, white paint and TiO\(_2\) nanoparticles, were chosen for further analysis.
Figure 39: Measured total reflectance of all investigated rear reflectors. [104]

**Angle dependent characterization of rear reflectors**

Second, the angle dependent reflectance in air was measured to compare the different scattering distributions of the diffuse rear reflectors. In addition, scanning electron microscopy (SEM) imaging was done. Figure 40 shows the SEM image of a) the backsheet, b) the white paint and c) the TiO$_2$ nanoparticles. The white paint also contains TiO$_2$ particles, but the SEM picture shows that they are dispersed in a binder. The TiO$_2$ nanoparticles in c) were deposited without an additional binder. Figure 40 d) shows the angularly resolved reflectance of the three reflectors for normal incidence at a wavelength of 1000 nm. The reflectance curve of a perfect Lambertian scatterer is plotted as well. In order to be able to compare the reflectance distribution to the Lambertian scatterer, the total reflectance has been normalized to the total reflectance of the Lambertian scatterer, which corresponds to an equal area under the curves in Figure 40 d). Figure 40 e) shows the difference of each reflector compared with the Lambertian scatterer. All three diffuse rear reflectors scatter light similarly to the ideal Lambertian scatterer. For all investigated samples, especially in the case of the backsheet, the forward scattering is slightly higher while the scattering into large angles is slightly lower than in the Lambertian case. Nevertheless, all three reflectors can be regarded as good diffuse reflectors in air. [104]
Figure 40: a,b,c) SEM images of the backsheet, white paint and TiO$_2$ nanoparticles. d,e) Angle-resolved reflectance measurement of the three different diffuse rear reflectors for normally incident light. All curves have been normalized to the total reflectance of the Lambertian scatterer, which corresponds to an equal area under the curves. [104]

**Absorption enhancement in solar cell precursors due to rear reflectors**

Third, the absorption enhancement of a silicon wafer due to the different rear side reflectors was determined by measuring $R$ and $T$ and calculating $A = 1 - R - T$. Figure 41 shows the measured absorptance spectra for the three different surface morphologies and all different rear reflectors. As upper benchmark, the black dashed line indicates the Yablonovitch-Limit related to a Lambertian rear reflector calculated according to equation (16), with an assumed front reflectivity set on a fixed value taken from a photospectrometric measurement of each sample type. For the pp-system the highest absorptance is achieved with white paint or with TiO$_2$ nanoparticles. The absorptance of the systems with air + backsheet and air + mirror is lower. For both, tp- and tt-systems, the difference between the different rear reflectors is very small. Only a small absorptance enhancement in comparison to the case without rear reflector can be achieved for the tp textured wafers, while on the tt samples with reflectors the Yablonovitch limit is reached.
Experimental realization of light trapping structures

The photo current density values $J_{ph}$ corresponding to the absorptance data presented in Figure 41 are summarized in Figure 42. In contrast to the solar cells that will be presented in the subsequent section, the optical test samples featured no ARC layer. With an ARC, because of the higher transmission through the front surface, overall more photons reach the rear of the wafer, which enhances also the absolute value of the photocurrent density gain due to a rear reflector. Therefore, Figure 42 also shows the estimated photocurrent density that would have been reached with an ARC considering the higher transmission through the front surface. To estimate this, the measured absorptance was multiplied with a correction factor of $(1-r_{ARC})/(1-r_{noARC})$. $r_{noARC}$ is the surface reflectivity without antireflection coating and $r_{ARC}$ the surface reflectivity with the additionally considered antireflection coating. For the pp wafers a wavelength-dependent correction factor was calculated considering a SiN$_x$/MgF$_2$ double layer antireflection coating that has also been used for the solar cells in the subsequent section. For the tp and tt wafers the correction factor only weakly depends on the wavelength and therefore the actual reflectivity values (at 900 nm) of the solar cells used in section 5.1.3 have been used. Please note that the thicknesses of the antireflection coatings are not optimized for highest cell efficiencies, because these solar cells have been originally designed for experiments with upconverting materials [112]. [104]
Especially for the pp system, white paint and TiO$_2$ nanoparticles show the highest $J_{ph}$ enhancement. This can be explained by the redistribution of light into larger angles within the silicon than for the other investigated structures. A slightly higher gain is predicted for the white paint compared to TiO$_2$ nanoparticles. This might be caused by the parasitic absorption of the binder contained in the white paint that also contributes to the absorptance, which would not lead to current generation in the solar cell, but cannot be excluded in purely optical measurements. The tp-system benefits from all rear reflectors similarly and only by a small amount, no matter whether the rear reflector reflects diffusely or directly. The tt wafers suffer from higher overall transmission without any rear reflector compared to tp wafers \cite{111}, hence a higher $J_{ph}$ enhancement compared to the tp wafers can be observed. However, the gain for the tt wafers is also roughly equal for all kinds of reflectors. This is due to the fact that for tp and tt wafers the system can benefit from additional reflection at the rear, but not much from additional redistribution of light into different angles, which is already done at the textured front (and rear) surface(s). For wavelengths higher than 1150 nm, the measured absorptance can be even higher than the calculated Yablonovitch-limit, which can be caused by parasitic effects and light that is not coupled into the integrating sphere. Note that this does not indicate beyond-Lambertian light trapping. In order to distinguish parasitic absorption effects (as can be seen for example in the case of the backsheet at 1140 nm and higher wavelengths in Figure 41) and useful absorption in the silicon bulk, finally leading to a higher $J_{SC}$, electrical measurements as presented in the following section are needed. \cite{104}

### 5.1.3 Solar cells with diffuse rear reflectors

When different rear reflectors are applied to different solar cells, statistical variations of the solar cells themselves can obscure the effects due to the reflectors. Therefore, the diffuse rear reflector of one
solar cell was varied, and the IV- and EQE-curve was measured for each rear reflector. Mirror, black cardboard and backsheets can be easily removed and TiO$_2$ nanoparticles can be removed in water within an ultrasonic bath. White paint is not easily removable and therefore was used only in the last step. All measured JV characteristics demonstrate that the different reflector types do not harm the basic functioning of the solar cells. Voltage and fill factor were not significantly affected by the different reflector types. To reveal the light trapping effect of the different reflector types, Figure 43 shows the EQE measurements for the three solar cell geometries: pp, tp and tt. The same reflectors as in the optical experiments have been used and again, the Yablonovitch-limit for each solar cell type is added as reference. [104]

![EQE measurements for different solar cell geometries](image)

Figure 43: Results of the EQE measurements with the different rear reflectors for solar cells with different surface morphologies. For the pp-solar cells, white paint and TiO$_2$ nanoparticles show a significantly higher absorption enhancement compared to the backsheet and the mirror. For the tp-solar cells, all rear reflectors show a similar absorption enhancement, while the tt-solar cells benefit slightly more from white paint and TiO$_2$ nanoparticles as compared to the backsheet and the mirror. [104]

Qualitatively, the results presented in Figure 43 are in good accordance to the results obtained by the optical measurements: the pp-solar cells benefit significantly from a diffuse rear reflector, in particular white paint and TiO$_2$ nanoparticles lead to a significantly higher EQE enhancement compared to the other materials. The tp-solar cell already has good light trapping because of the textured front surface and the planar rear surface. The tp-solar cell benefits from a rear reflector but it is not relevant, which type of rear reflector. To facilitate a simple quantitative comparison, Figure 44 shows the short circuit
current density gains $\Delta J_{\text{SC}}$ between 900 and 1200 nm for the different rear reflectors in comparison to the black cardboard rear reflector. All values have been determined by integrating and weighting the EQE, not by IV-measurements. The results obtained from one single sample are displayed as a cross in Figure 44, indicating the deviation between identically processed samples. The colored bars represent the mean values. For a comparison of the optical and electrical results, the gray bars represent the gain $\Delta J_{\text{ph,ARC}}$ obtained from the optical measurements including the estimation of an ARC (as presented in Figure 42). There are different effects causing deviations between the optical and electrical measurements: first, comparing photo current densities with short circuit current densities assumes a carrier collection efficiency of 100%. The cells feature an IQE above 0.99 in the visible wavelength range, which indicates a very high collection efficiency. However, an IQE losses might contribute to the overall deviation. Second, the (parasitic) absorption within the rear reflector materials is included in the optically measured absorptance, and therefore contributes to a higher $\Delta J_{\text{ph,ARC}}$ estimated from those measurements, but in fact does not contribute positively to the EQE. Additionally, the solar cells feature a metal front grid leading to shading and a metal rear grid slightly reducing the effective area of the reflector. With respect to these effects, the optical measurements can be understood as upper limits for the short circuit current density gain that could be reached. In summary, while the precise quantitative values predicted by optical measurements slightly differ from the final characterization with solar cells, the qualitative results of optical and electrical measurements are in good accordance to each other. [104]
Experimental realization of light trapping structures

Figure 44: Current density gain (based on EQE-measurements) in comparison with a black reflector at the rear. The $J_{SC}$ and $J_{ph,ARC}$ were integrated between 900 and 1200 nm. The colored bars represent the mean value of the electrical measurements. The gray bars represent the calculated photo-current gain with estimated ARC. The crosses indicate individually measured solar cells.\[104\]

All current density gains, obtained either by optical measurements ($\Delta J_{ph}$) with solar cell precursors or by EQE measurements with fully processed solar cells ($\Delta J_{sc}$) are summarized in Table 4. One has to keep in mind that the solar cells have been originally designed for upconversion experiments and thus the absolute values $J_{SC}$ are not optimized. The gain $\Delta J_{SC}$ for the pp-solar cells accounts for 0.9 mA/cm$^2$ for the backsheet and over 1.7 mA/cm$^2$ for white paint and TiO$_2$ nanoparticles. Compared with the optical samples in Figure 42, the solar cell with white paint and TiO$_2$ nanoparticles show a 0.8 mA/cm$^2$ lower current gain. This is caused by the effects discussed above. The difference in the gain for the backsheet is smaller than for white paint and TiO$_2$ nanoparticles, although the backsheet has a higher parasitic absorption (see Figure 41); this is caused by the generally lower light trapping due to the air gap. The mirror shows similar results as the backsheet. For the tp-solar cells, the gain deduced from the electrical and optical measurements is very similar and lies within the variation of the individual measurements. For the tt-solar cells, a generally lower influence of parasitic absorption in comparison with the pp-solar cell can be observed. This is caused by the textured surfaces and the generally better light trapping. White paint and TiO$_2$ nanoparticles show the highest current gain for the tt-solar cell (about 1 mA/cm$^2$). The mirror and the backsheet show a similar gain of 0.7 and 0.8 mA/cm$^2$. The values in brackets are taken from [111]. Qualitatively, those values fit to the results obtained in this work. However, the gain observed for tt cells is significantly smaller than reported in [111], and the
overall photo current density for tt cells with diffuse rear reflector is not higher than for tp cells with a diffuse rear reflector. [104]

Table 4: $\Delta J_{ph,ARC}$ and integrated $\Delta J_{SC}$ between 900 and 1200 nm. For integrated $J_{SC}$ between 280 and 1200 nm, the mean value of the measurements is shown, corresponding to the colored bars in Figure 44. The gain was calculated in comparison to black cardboard as rear reflector for both, the electrical and optical measurements. The values in brackets are the values reported by Frank et al. [111].

<table>
<thead>
<tr>
<th>$J_{SC}$ [mA/cm²] 280 - 1200nm with black rear reflector</th>
<th>planar/planar (pp)</th>
<th>texture/planar (tp)</th>
<th>texture/texture (tt)</th>
</tr>
</thead>
<tbody>
<tr>
<td>rear reflector</td>
<td>$\Delta J_{ph}$</td>
<td>$\Delta J_{SC}$</td>
<td>$\Delta J_{ph}$</td>
</tr>
<tr>
<td>air + mirror</td>
<td>1.4</td>
<td>1.0</td>
<td>0.4</td>
</tr>
<tr>
<td>air + backsheet</td>
<td>1.5</td>
<td>0.9</td>
<td>0.4</td>
</tr>
<tr>
<td>white paint</td>
<td>2.6 (2.3)</td>
<td>1.8</td>
<td>0.5 (0.3)</td>
</tr>
<tr>
<td>TiO$_2$ nanoparticles</td>
<td>2.5</td>
<td>1.7</td>
<td>0.4</td>
</tr>
</tbody>
</table>

To summarize this section about simple diffuse rear reflectors, Table 4 can be seen as a benchmark for all light trapping structures for wafer based crystalline silicon solar cells. Every novel light trapping concept including more complex structures and processes has to compete with these simple diffuse rear reflectors presented. The following two sections about nanoimprinted binary gratings and about sphere gratings present two such concepts that allow for even higher light trapping than simple diffuse rear reflectors.

5.2 Binary gratings

As already indicated in Figure 8 and described in the introduction, diffractive structures at the rear are promising for realizing long light path lengths due to diffraction into oblique orders. Also detailed simulation results presented in chapter 6 demonstrate that binary gratings at the rear allow for very good light trapping. The aim of this work was the integration of diffractive structures into fully processed solar cells following the EPOS (electrically planar, optically structured) concept and the demonstration of a real benefit for silicon solar cells due to gratings at the rear. To reach an efficiency enhancement due to a rear structure on final device level, three key challenges have to be addressed: First, the electrical passivation quality must not be decreased in order to reach the same or an even higher voltage compared to a reference solar cell. Second, electrical contacts that allow for low series resistance losses have to be developed to enable the same or an even higher fill factor. And third, the grating has to increase the absorption in the silicon solar cell in order to increase the current. To address all three challenges, a complete process chain combining the grating fabrication itself and the solar cell processing was developed. The following section 5.2.1 describes these processes before optical and finally electrical results are presented in 5.2.2 and 5.2.3.
5.2.1 Process development and process chain

The process development with regard to the binary grating fabrication itself (nanoimprint lithography, etching) was done by Nico Tucher [65] on the basis of previous works at Fraunhofer ISE (mainly by Hauser et al. [113–115]). I was responsible for processes and tests for the integration into wafer based silicon solar cells (passivation tests, contact formation) in cooperation with Nico Tucher. Therefore, the grating fabrication processes are presented only briefly as basis for the more detailed description of the integration processes.

Process chain of grating fabrication

The binary gratings have been realized via nanoimprint lithography (NIL) and subsequent plasma etching. The basic process chain is sketched in Figure 45: For the fabrication of stamps for the NIL process, a master structure is created by interference lithography and replicated into a polydimethylsiloxane (PDMS) material by cast molding. The EVG-Smart-NIL technology [116] is used to press the PDMS stamp into a photoresist. The resist is cured by a UV-exposure and afterwards the stamp is demoulded and a patterned resist layer remains on the substrate. This patterned resist layer serves as an etching mask featuring the diffractive grating structure. By anisotropic reactive ion etching at an Oxford Plasmalab 133, using SF₆ and O₂ as etching gases, the grating structure is transferred to the silicon substrate. A detailed description of NIL in general can be found in [117]. The different process steps during the fabrication of diffraction gratings via nanoimprint lithography are explained in [114].

![Figure 45: Schematic process chain of nanoimprint lithography (NIL) for structuring a silicon substrate. The PDMS stamp (green) was replicated from a master structure fabricated with interference lithography.](image)

For future industrial applications of such a process chain in the field of photovoltaics, important issues like stamp life time and detailed process development are addressed in [65].
Passivation concept

In order to realize the EPOS concept, it is not possible to directly pattern the silicon bulk at the rear of the solar cell. Experimental tests to effectively passivate patterns created with the plasma etching process used at Fraunhofer ISE have not been successful yet. Therefore, a 10 nm thin Al₂O₃ layer was used as passivation layer and an additional layer was needed for the patterning. This additional layer has to fulfill several requirements. First, the deposition may not affect the passivation quality of the Al₂O₃ layer. Second, it should feature a refractive index close to the silicon bulk in order to reach good coupling efficiencies of the diffraction orders. Third, it should feature no absorption in the near infrared where light reaches the rear of the solar cell and the grating. From an optical point of view, amorphous silicon (a-Si) is perfectly suitable, as the refractive index is very similar to c-Si and the absorption coefficient in the NIR is close to zero due to the higher bandgap of a-Si in comparison to c-Si. In first experiments, PECVD depositions of a-Si have been used, but this led to strong adhesion problems when the a-Si layer was thicker than 100 nm. For an efficient grating, however, thicknesses in the range of at least 200 nm are required [118] and therefore alternative deposition methods had to be investigated. With sputtering of a-Si, thick layers with good adhesion were deposited and life time samples indicated that there are no significant detrimental effects to the Al₂O₃ passivation layer due to the sputtering process or any of the grating fabrication steps. All following results were obtained with grating structures in a sputtered a-Si layer as depicted in Figure 47.
Figure 47: Sketch of a silicon solar cell (front structure including emitter, ARC etc. and contacts not shown) with an additional, binary a-Si grating at the rear of the cell. A thin Al₂O₃ passivation layer separates the optical and electrical properties at the rear. The red light paths indicate the possible light path length enhancement due to diffraction.

**Contact formation**

As neither the passivation layer (Al₂O₃) nor the grating structure (a-Si) is conductive, local contacts have to be applied. This means, that the grating structure and the passivation layer have to be opened locally allowing for a direct contact of the rear metallization to the silicon bulk (or the back surface field). Two routes for such local contacts have been applied and adapted to the grating structure within this work.

**Photolithography + etching steps**

The first route is based on photolithography (PL) and different etching steps followed by aluminum evaporation. An aluminum evaporation on top of the grating structure would lead to a patterned metal contact and thus to strong parasitic absorption within the metal. Therefore, this route requires an additional step that planarizes the grating with a low-refractive index material. For this planarization, SiO₂ nanoparticles deposited via spin coating were chosen. Details about the planarization process and its beneficial impact on parasitic absorption losses have been presented in [119]. On top of the complete rear structure (Al₂O₃, patterned a-Si, SiO₂), a resist layer is spincoated and photolithographically structured as etching mask. Then, the three underlying layers have to be opened. A plasma etching process based on SF₆ and O₂ was found to etch the nanoparticle based SiO₂ layer and at the same time the a-Si grating. The Al₂O₃ layer serves as perfect etch stop and thus the exact etching time is not very critical and a possible damage of the silicon bulk is avoided. Subsequently, the remaining Al₂O₃ layer can be removed in a short hydrofluoric acid (HF) based wet-chemical etching step. Figure 48 depicts this process chain.
5 Experimental realization of light trapping structures

Figure 48: Schematic process steps for the contact openings with a rear binary grating. In the first step, a resist layer (red) is structured by photolithography to define the point contact geometry. In the second step, a plasma etching process based on SF₆ and O₂ is used to etch the SiO₂ planarization layer and the a-Si grating. In step 3, the Al₂O₃ passivation layer is opened with HF and in step 4 Al is evaporated to form the contact.

For point contact openings, this process sequence is difficult to monitor, as the main way of characterizing and controlling successful contact openings is to look at cross sections in the SEM. Therefore, line contact openings were processed in a test batch to develop a working process for the solar cell batch presented in 5.2.3. For further simplification no grating was fabricated for this test batch but a homogeneous, 300 nm thick a-Si layer was deposited. Figure 49 shows the line openings after the plasma etching process. The clear under-etching shows that Al₂O₃ works as etch barrier and indicates an overestimation of the etching time.

Figure 49: SEM cross section pictures of line shaped contact openings as pretests for point contacts in solar cells. On top of the structure the photo resist that endures the etching processes can be seen. Below the photoresist the spin coated SiO₂-layer (planarization) and the amorphous silicon layer can be seen. There is a significant etching below the photoresist which shows that the Al₂O₃ layer works as an etch barrier. The Al₂O₃ layer is invisible here due to its thickness of only 10 nm. The c-Si remains without damage and can be contacted by subsequent evaporation of aluminum. [120].

After the contact opening process an evaporation of Aluminum is used to form the electrical contact to the silicon bulk. To reach a sufficient lateral conductivity underneath the contact points and thus low series resistance losses, an aluminum doped back surface field can be used as depicted in the schematic solar cell sketch in Figure 51.
**Foil-LFC**

As second method a foil-based laser fired contacts (LFC) process was investigated. Foil-based LFC has been developed at Fraunhofer ISE for contacting p-type cells passivated at the rear [121,122]. An aluminum foil is attached to the rear surface and locally melted through the grating structure and the thin passivation layer using a laser. With an adequate laser process, point contacts that provide an electrical contact from the aluminum foil to the silicon bulk can be realized. The electrical contact points also provide the mechanical adhesion between the foil and the solar cell. At the rest of the interface, there is a small air gap between the foil and the substrate. In combination with the diffractive grating, this process has several advantages compared to the route based on photolithography and etching. First, an air gap remains between the aluminum foil and the solar cell in between the LFC points minimizing parasitic absorption in the aluminum and making the additional planarization layer unnecessary. Second, the higher refractive index contrast between a-Si and air (compared to a-Si and SiO₂) leads to higher diffraction efficiencies. Third, the process is much faster and comprises just one process step in contrast to the numerous steps of the PL-based etching route. For this work, the LFC process was adjusted to the layer system including the grating by Martin Graf, Fraunhofer ISE. Test samples with fully metallized front and a boron doped back surface field with the grating structure at the rear have been prepared. A green laser with a wavelength of 532 nm was used, the laser power has been adapted and the number of laser pulses per point was increased to three. With a square array of point contacts using a pitch of 700 µm, resistance measurements through the whole structure from the fully metallized front to the point-contacted, foil-metalized rear have been conducted. The measured resistance values are in the range of the expected spreading resistance, hence no significant contact resistance has been determined. This measurement is quantitatively not very reliable but gives a strong hint for low contact resistances. Furthermore, a very good mechanical adhesion of the foil was observed. With the pitch of 700 µm and a contact point diameter of approximately 40 µm, on 99.7% of the total rear area, the grating structure is not affected by the contact process, which is very important from an optical point of view. [120]

### 5.2.2 Optical characterization of binary gratings

At the beginning of this work already several optical measurements of similar grating structures at the rear of silicon wafers had been published. Especially the works by Hauser et al. [113,114] and Mellor et al. [55,87] demonstrated significant absorption enhancements for nanoimprinted line and crossed gratings at the rear of silicon wafers in comparison to flat rear surfaces. The main focus within this work was the integration of such structures into working devices and therefore the structure as described in Figure 51 was developed. Prior to the processing of solar cells, optical test samples were fabricated together with the test samples for passivation and contact formation. Figure 50 shows photospectrometric measurements of 250 µm thick silicon wafers with a crossed grating in a-Si at the
rear as indicated in Figure 51. For reference, the absorptance of a both side planar silicon wafer is also shown.

![Absorptance and Absorbance Gain Graphs](image)

**Figure 50:** Left: Absorptance of a silicon wafer with a binary crossed grating and/or an Al-foil attached by a LFC process at the rear. Right: Absolute absorptance gain for the same samples with respect to the planar reference. A significant absorptance enhancement peak between 1050 nm and 1150 nm is visible. Absorption at wavelengths larger than 1200 nm indicates parasitic absorption as the absorption coefficient of c-Si is close to zero in this wavelength range.

Figure 50 shows a clear absorption enhancement due to the grating in the near infrared. A quantitative analysis of such optical measurements is questionable as useful absorption within the c-Si and parasitic absorption in any other part of the system cannot be separated. However, some qualitative conclusions can be drawn based on Figure 50. Compared to a planar reference without any rear reflector (equivalent to a black rear reflector due to the black housing of the photospectrometer Cary 5000i), both, the Al-foil and the a-Si grating individually lead to a significant absorption enhancement. The combination of both, which is the case relevant for the final solar cells, shows the highest absorption enhancement with close to 50% absolute at 1100 nm. Considering the significant absorption even at 1300 nm, the Al-foil and the a-Si grating feature parasitic absorption. Note that quantitatively precise absorptance measurements of low absorbing, structured sheets with an integrating sphere via 1-R-T can be difficult as light can be guided to the edges of the sample and small measurement uncertainties sum up to large relative errors due to the subtraction of R and T from 1. A good description about these issues can be found in [90]. However, the qualitative conclusions for the measurements in Figure 50 are still valid. A way of separating useful and parasitic absorption quantitatively is the analysis of the EQE in a solar cell as presented in the following section.

### 5.2.3 Solar cells with binary gratings

Based on the passivation concept and the two concepts for contact formation, Figure 51 schematically shows the developed solar cell concept. The fabricated solar cells feature a PERT (passivated emitter and rear totally diffused) cell structure. As base material, 4 inch float zone p-type silicon wafers with a resistivity of 1 Ωcm and a thickness between 100 and 250 μm were used. On each of the 24 wafers in
the batch, seven cells with an active area of 2x2 cm² were fabricated. A 120 Ω/sq front side emitter was realized by phosphorous diffusion and a 100 Ω/sq. back surface field by boron diffusion. A 105 nm thick SiO₂ dielectric passivation layer was grown at the front. Despite its very low refractive index, this SiO₂ layer also serves as antireflection coating (ARC). The focus in this experimental demonstration of rear gratings was near infrared light trapping and hence the non-optimum front ARC is of minor importance. It was chosen for reasons concerning process stability and could be replaced in principal by optically superior ARC layers or multilayers like presented in section 4.1. Photolithography, metal evaporation and light induced plating were used to form the front side metal grid [123]. The grating at the rear was realized as described in the previous sections in a-Si with a thin Al₂O₃ passivation layer. SEM pictures of the grating are shown in Figure 46. Both contact formation processes have been tested for the 250 μm thick solar cells. For the thinner cells, only foil-based LFC was used after the principle functioning of the Al-foil was demonstrated for the 250 μm thick solar cells. Two types of reference solar cells were fabricated for 250 μm thick solar cells: cells with a 100 nm thick SiO₂ layer instead of the a-Si grating (similar to a standard PERC) and cells with an a-Si and SiO₂ layer stack where the a-Si remains unstructured. [124]

Figure 51: Schematic structure of the realized solar cell concept: a p-type silicon solar cell with passivated emitter at the front, featuring a binary crossed grating at the rear for enhanced light trapping of near infrared light. For local contacts either an aluminum foil was applied (left) or aluminum was evaporated into predefined local contact openings. The front was either planar (like depicted here) or pyramidally textured. [124]

As a combination of a pyramidal front texture with a grating at the rear is a promising approach for combining low reflection losses and enhanced near infrared light trapping, also cells with textured front surface have been processed. Therefore, on each wafer, two of the seven solar cells have been textured at the front with inverted pyramids. Table 5 gives an overview of the processed solar cell types with abbreviations used in the following evaluation of the results.
Table 5: Overview of the processed solar cells. For 250 µm cell thickness, 2 different contact formation processes (foil-LFC and PL + etching) and two different reference types (just SiO$_2$ layer or SiO$_2$ + unstructured a-Si) have been tested. For all thinner cells, only foil-LFC and SiO$_2$ at the rear of the reference cell have been used. All listed solar cells are planar at the front (eg. pp250). For each type also cells with an inverted pyramids texture at the front surface were processed (eg. tp250) with the same properties apart from that.

<table>
<thead>
<tr>
<th>Textures front/rear</th>
<th>Cell thickness [µm]</th>
<th>Detailed rear side structure</th>
<th>Abbreviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Planar/planar</td>
<td>250</td>
<td>100 nm SiO$_2$, Foil-LFC</td>
<td>pp250</td>
</tr>
<tr>
<td>Planar/planar</td>
<td>250</td>
<td>100 nm SiO$_2$, PL + etching</td>
<td>pp250, PL + etching</td>
</tr>
<tr>
<td>Planar/planar</td>
<td>250</td>
<td>200nm unstructured a-Si + 100 nm SiO$_2$, Foil-LFC</td>
<td>pp250, with a-Si layer</td>
</tr>
<tr>
<td>Planar/planar</td>
<td>250</td>
<td>200nm unstructured a-Si + 100 nm SiO$_2$, PL + etching</td>
<td>pp250, PL + etching, with a-Si layer</td>
</tr>
<tr>
<td>Planar/grating</td>
<td>250</td>
<td>Grating, Foil-LFC</td>
<td>pg250</td>
</tr>
<tr>
<td>Planar/grating</td>
<td>250</td>
<td>Grating, PL + etching</td>
<td>pg250, PL + etching</td>
</tr>
<tr>
<td>Planar/planar</td>
<td>150</td>
<td>100 nm SiO$_2$, Foil-LFC</td>
<td>pp150</td>
</tr>
<tr>
<td>Planar/grating</td>
<td>150</td>
<td>Grating, Foil-LFC</td>
<td>pg150</td>
</tr>
<tr>
<td>Planar/planar</td>
<td>100</td>
<td>100 nm SiO$_2$, Foil-LFC</td>
<td>pp100</td>
</tr>
<tr>
<td>Planar/grating</td>
<td>100</td>
<td>Grating, Foil-LFC</td>
<td>pg100</td>
</tr>
</tbody>
</table>

For each surface texture combination (planar and textured front, planar and grating rear), calibrated JV and EQE measurements have been conducted by Fraunhofer ISE CalLab for one particular solar cell. Subsequently, for all cells the JV- and EQE-characteristics was measured using the analysis system LOANA (pv tools) and an AM 1.5g STC solar simulator (Oriel, class B) using the calibrated solar cells as reference cells to ensure a precise measurement of the short circuit current density. Especially the comparison of solar cells with quite different EQEs in the near infrared requires the use of similar solar cells with regard to the spectral sensitivity as reference cells in order to avoid large spectral mismatch errors. [124]

**Solar cells with planar front**

For the solar cells with a thickness of 250 µm, the number of investigated variations is higher than for thinner cells (see Table 5). Therefore, the results for all cells with planar front are presented in two steps. First, the results shown in Figure 52 for all cells with a thickness of 250 µm are discussed. Afterwards, the results for different cell thicknesses are evaluated. The $J_{SC}$ results in Figure 52 demonstrate that there is a considerable short circuit current density gain of 1-2 mA/cm$^2$ due to the grating. All reference solar cells (pp) feature a quite similar current, which indicates similar optical properties of the rear of all reference solar cells, regardless of the metallization. Concerning the
voltage and fill factor, there are no clear differences between cells with grating and reference cells without grating. This indicates that the introduction of the grating to the solar cell does not significantly affect the passivation quality and the contact resistances. This confirms the investigations with life time samples and the contact formation experiments described above. However, there are some differences between the different reference solar cells. The cells contacted with foil-LFC show a slightly lower voltage and fill factor. This, however, cannot be confirmed for the cells with a grating at the rear. Overall, the cells with grating show the highest efficiencies of up to 19.0% and thus, Figure 52 demonstrates the successful realization of electrically planar, but optically structured (EPOS) solar cells.

Figure 52: Measured \( J_{SC} \), \( V_{OC} \), FF and efficiency \( \eta \) of crystalline silicon solar cells with planar front surface and planar (pp) or grating rear (pg). Two different contact formation processes (Foil-LFC and PL + etching) and two different reference types (with or without a-Si layer) are shown. Crosses show the results for all individual cells, the boxplots show median and 25/75 percentile.

For all thinner solar cells (150 µm, 100 µm), only foil-LFC was used and only references with a SiO\(_2\) layer were fabricated. Figure 53 shows the measured cell parameters for all three thicknesses and each texture combination for the Al-foil contacts. Note that the values for the 250 µm thick solar cells

---

1 Measured by Fraunhofer ISE Callab. Cells in Figure 52 are measured at an AM 1.5g STC solar simulator (Oriel, class B) using the calibrated solar cells as reference cells. Therefore minor differences, e.g. efficiencies of up to 19.1% appear.
(depicted in orange) are the same as presented in Figure 52. The considerable short circuit current density gain of 1-2 mA/cm² due to the grating can be seen again, further increasing with decreasing cell thickness. This increase for thinner cells indicates that the gain is really caused by enhanced light trapping in the near infrared, as for thinner cells more light reaches the rear and light trapping properties gain in importance. Reconfirming the results for cells with a thickness of 250 µm, voltage and fill factor are not significantly affected by the grating.

Figure 53: Measured $J_{SC}$, $V_{OC}$, FF and efficiency $\eta$ of crystalline silicon solar cells with planar front surface and planar (pp) or grating rear (pg) and three different cell thicknesses (250, 150 and 100 µm). Crosses show the results for all individual cells, the boxplots show median and 25/75 percentile. All shown cells have Al-foil based LFC contacts at the rear. [124]

To investigate the current density gain due to the grating in more detail, EQE measurements of the best cells of each group of cells have been conducted. Figure 54 shows the EQE measurements for all 250 µm thick solar cells.
Figure 54: Measured EQE of 250 µm thick solar cells with and without a binary grating at the rear. The four different types of reference solar cells without a grating show a very similar EQE. The cells with a grating show a clearly enhanced EQE in the NIR, regardless of the contact formation process.

For the different solar cell thicknesses, the EQE results are shown in Figure 55. Additionally, the EQE gain due to the grating is calculated by subtracting the EQE of a cell without grating from the EQE of a cell with grating. Weighted with the AM1.5g spectrum, the EQE measurements correspond to a photo current density gain of 1.2 mA/cm² (250 µm), 1.6 mA/cm² (150 µm) and 1.8 mA/cm² (100 µm), which is in good agreement to the JV measurements presented in Figure 53.
Figure 55: Measured EQE gain due to grating integration at the rear for a planar solar cell front. For thinner solar cells the gain increases at smaller wavelengths. Weighted with the AM1.5g spectrum the three curves correspond to a short circuit current density gain of 1.2 mA/cm$^2$ (250 µm), 1.6 mA/cm$^2$ (150 µm) and 1.8 mA/cm$^2$ (100 µm).

[124]

Solar cells with textured front and binary grating at the rear

On each of the wafers, two of the seven cells have been textured at the front with inverted pyramids. Thus, the total number of cells in the different sub-groups is very low and a statistical evaluation has a limited significance. Nevertheless, Figure 56 shows the box plots for all cell parameters determined by JV-measurements. The clear trend in $J_{SC}$ that was visible for cells with planar front surface cannot be seen here. The deviations between individual cells are larger and mean values may be interpreted with caution due to the low number of cells. At least the majority of cells with grating (tg) show a lower $V_{OC}$ and FF in comparison to the references with planar rear (tp). However, in the previous section the results for cells with planar front surface already demonstrated that the additional processes related to the grating fabrication do not cause any loss in $V_{OC}$ or FF. As the cells with planar and textured front surface are processed on the same wafers and thus see identical processes (except of the KOH-texturing), these results seem to be in contradiction to each other. It is unclear, why there is a detrimental effect just in the case of front side texturing. Presumably, one of the steps in the solar cell process (not in the grating fabrication) works differently for textured and planar samples. As both front side types were processed on the same wafers, no individual adaption of processes was possible. Because no samples for measuring minority carrier life times, contact resistances etc. after each process step have been added to the solar cell batch, a detailed analysis where this difference
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originates from is beyond the scope of this work. However, these issues are not considered to be fundamental due to the results obtained with cells with planar front.

Figure 56: Measured $J_{SC}$, $V_{OC}$, FF and efficiency $\eta$ of crystalline silicon solar cells with inverted pyramids at the front surface and planar (tp) or grating rear (tg) and three different cell thicknesses (250, 150 and 100 µm). Crosses show the result for all individual cells, the boxplots show median and 25/75 percentile. All shown cells have Al-foil based LFC contacts at the rear side.

In order to look for possible influences related to the grating without looking at the large deviations between individual cells, Table 6 shows the $JV$ measurement results of the best cells in each group.

Table 6: Summarized $JV$ data of the best cells of each group. “tp” or “tg” mean textured front (inverted pyramids) and planar rear or grating rear, followed by the cell thickness.

<table>
<thead>
<tr>
<th></th>
<th>$J_{SC}$ [mA/cm$^2$]</th>
<th>$V_{OC}$ [mV]</th>
<th>FF</th>
<th>$\eta$ [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>tp 250*</td>
<td>39.5</td>
<td>671.1</td>
<td>0.786</td>
<td>20.8</td>
</tr>
<tr>
<td>tg 250</td>
<td>39.3</td>
<td>669.2</td>
<td>0.760</td>
<td>20.0</td>
</tr>
<tr>
<td>tg 250$^1$</td>
<td>39.5</td>
<td>670.5</td>
<td>0.803</td>
<td>21.2</td>
</tr>
<tr>
<td>tp 150</td>
<td>39.5</td>
<td>676.3</td>
<td>0.782</td>
<td>20.9</td>
</tr>
<tr>
<td>tg 150</td>
<td>39.7</td>
<td>675.2</td>
<td>0.789</td>
<td>21.1</td>
</tr>
<tr>
<td>tp 100</td>
<td>39.4</td>
<td>673.8</td>
<td>0.779</td>
<td>20.7</td>
</tr>
<tr>
<td>tg 100</td>
<td>39.5</td>
<td>674.0</td>
<td>0.785</td>
<td>20.9</td>
</tr>
</tbody>
</table>

* measured by Fraunhofer ISE Callab

$^1$ contact openings via PL and etching like depicted in Figure 48, all other cells contacted via foil-LFC
The measured $JV$ data do not show any significant changes due to the grating, but vary statistically. Note again that the number of cells in each group here is below 10. Regarding the current density, slight changes in the thickness of the ARC or slight inhomogeneities in the metallization can overcompensate any possible grating effect. The grating effect can, however, be revealed in the EQE measurement in the near infrared. Figure 57 shows the measured EQE gain due to the grating between 800 and 1200 nm. The gain is significantly smaller than in the case of a planar front, because the front pyramids already lead to a light path length enhancement themselves. Nevertheless, the grating is still beneficial and causes a small current density gain of about 0.3 mA/cm$^2$. Thus, low front side reflection and improved light trapping can be combined.

![EQE Gain vs Wavelength](image)

Figure 57: Measured EQE gain due to a grating at the rear for solar cells featuring a front texture with inverted pyramids. For 150 µm thick solar cells the gain increases at smaller wavelengths and gets larger in total compared to 250 µm thickness. For 100 µm cell thickness the gain is smaller, which is attributed to processing issues. Weighted with the AM1.5g spectrum, the three curves correspond to a photo current density gain of 0.26 (250 µm), 0.34 (150 µm) and 0.24 mA/cm$^2$ (100 µm). [124]

### 5.2.4 Comparison to simulations

The optical properties of all fabricated solar cells can in principle be simulated using the methods described in chapter 3. Within this section, OPTOS simulations are compared with the previously described measurements. Besides the basic physical understanding and validation, the purpose of such a comparison is the identification of possible loss mechanisms and options for a further optimization of the fabricated structures.
To run an OPTOS calculation corresponding to the fabricated solar cells, redistribution matrices for the front and rear surfaces are needed. The front surface is either planar or textured with inverted pyramids, in both cases featuring a 100 nm thick SiO$_2$ passivation and ARC layer. As already shown in section 3.2.5, such matrices can be calculated using TMM and ray tracing. For the rear matrices, RCWA is used and grating parameters in accordance to the SEM picture depicted in Figure 46 are used: round pillars of a-Si with a period of 1 µm, a pillar diameter of 800 nm and a pillar height of 180 nm. The 10 nm thin Al$_2$O$_3$ passivation layer and the residual a-Si layer thickness of 120 nm were also included in the redistribution matrix calculation. A further important parameter for the simulation that is, however, difficult to determine, is the air gap thickness. Measurements with SEM cross sections, also produced by a focused ion beam, influence the air gap thickness and thus are not reliable. At the contact points, which cover 0.3 % of the rear, the air gap thickness is zero. As the contact points are separated by several hundred micrometers, an air gap thickness of at least a few hundred nanometers seems to be a reasonable assumption. Additionally, the thickness is varying between zero at the contact points and some maximum value in between. Thus, choosing some specific value for the air gap thickness would not be reasonable and therefore, the air gap was treated incoherently, instead. Such an incoherent coupling can be accounted for by calculating an effective interface matrix as presented in section 3.2.4. The interface from silicon to air containing the grating structure and the interface from air to Al are combined into one effective interface. The air gap thickness in this case has no influence. Detailed, purely wave-optical simulations showed that such an incoherent coupling is equivalent to averaging over different air gap thicknesses in fully coherent calculations, when the air gap thickness is at least a few hundred nm. Further details about the comparison of fully coherent rear side matrices with effective matrices can be found in [65]. For all following simulations, the incoherent coupling was chosen. The detailed simulations indicated also that there would be additional parasitic losses due to near field coupling into the aluminum, if the air gap thickness was smaller than a few hundred nanometers.

Figure 58 shows the OPTOS simulation result for a solar cell with planar front and a binary grating at the rear in comparison to the EQE of the fabricated solar cell (same curve as in Figure 55). To account for the front metal grid, which is not considered in the redistribution matrix calculation of the front surface, the simulated absorptance curve has been corrected by -3% rel. The good agreement of simulation and measurement in the short wavelength range indicate a correct description of the solar cell’s front surface. Regarding the rear, however, the simulation indicates a significantly larger absorptance gain than measured in the final solar cell. One possible explanation would be that the air gap thickness - at least at some parts of the rear - is thinner than a few hundred nanometers and would have to be treated coherently. As explained above, this is considered to be unlikely. The second, more likely reason for the deviation is significant parasitic absorption in the rear structure as already indicated by optical measurements in section 5.2.2. Two main sources of parasitic absorption have been identified: parasitic absorption within the a-Si, e.g. due to defect states, and parasitic absorption...
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at the interface from air to Al, which was assumed to be perfectly planar in the simulation. Accounting for such a loss mechanism, the redistribution matrix of the rear surface can be multiplied by a factor smaller than one, e.g. 0.9. Such a factor of 0.9 corresponds to an additional parasitic absorption of 10% for each interaction at the rear. This allows for testing the assumption of parasitic absorption without knowing or modeling the exact loss mechanism. Figure 58 (a) shows the simulated absorptance for three different factors: 1.0 (corresponding to the original matrix), 0.9 and 0.8. Obviously, with a factor of 0.9 the simulation results can be matched. Figure 58 (b) shows, that the same factor of 0.9 also leads to good agreement for the thinner solar cells, which further indicates that the original difference between simulation and measurement is caused by parasitic absorption at the rear of the cell [123]. Figure 58 (c) shows that also for cells with textured front, a good agreement with this simulation approach can be reached. Both, simulation and measurement show small current density gains of at most 0.5 mA/cm² for solar cells textured at the front. To further evaluate the exact origin of parasitic absorption, an additional set of samples would be necessary. Definitely, future work on gratings for the rear, following the process chain presented here, should focus on parasitic absorption within the rear structure.
Figure 58: (a) OPTOS calculations in comparison with EQE measurements for a 250 µm thick cell with planar front and planar or grating rear side. A factor of 0.9 for the rear side redistribution matrix (means 10% losses at each interaction with the rear side) accounts for a parasitic absorption loss at the rear side without exactly knowing its origin. It leads to a result similar to the measurement. (b) shows the simulated (including 10% losses) and measured EQE gain due to the grating for a planar front side, (c) for a textured front side. [123]

5.3 Sphere gratings

In the following section, I describe a further diffractive structure to improve light trapping: sphere gratings. The name refers to its basic constituent, monodisperse silica (SiO₂) spheres. “Monodisperse” means that all silica spheres feature the same diameter. The work on sphere gratings was started at Fraunhofer ISE by Voisin et al. [125] and Janz et al. [126]. Based on these initial investigations, I examined the fabrication of sphere gratings within my diploma thesis [127]. Within this work, I aim for an integration of sphere gratings into fully processed, high-efficiency silicon solar cells, while simultaneously improving the optical properties and the fabrication processes. The development of a solar cell process chain including sphere gratings was done in close collaboration with Benjamin G. Lee during his one-year stay as guest scientist at Fraunhofer ISE and led to a joint publication [128]. Identical to the binary gratings, three key challenges have to be overcome for a successful integration
of sphere gratings into high-efficiency silicon solar cells: the electrical passivation must be ensured, good electrical contacts have to be realized and the absorption in the silicon bulk has to be enhanced. To address all three challenges, a process chain combining the grating fabrication itself and the solar cell processing aiming for an EPOS cell, was developed. The following section 5.3.1 describes details about the experimental processes. The optical and electrical results are presented in 5.3.2 and 5.3.3. Section 5.3.4 shows a comparison of the results with sphere gratings to simulations and identifies options for further improvements.

5.3.1 Process development and process chain

Process chain of grating fabrication

For the grating itself, a two-step process has been developed. First, a dense monolayer of spheres is deposited via spin coating and, second, the voids in between the spheres are filled with a high refractive index material. The refractive index contrast between the spheres (SiO$_2$, $n \approx 1.5$) and the high refractive index matrix (TiO$_2$, $n \approx 2.4$, or Si, $n \approx 3.5$) leads to diffraction. In the following, the two steps of the production process are presented.

Spin coating of SiO$_2$ spheres

The monodisperse SiO$_2$ spheres are fabricated by a wet-chemical procedure based on the Stöber process [129] and can be transferred to an arbitrary solvent (unless this solvent dissolves SiO$_2$). Within this work, commercially available SiO$_2$ spheres in an aqueous solution have been used$^1$. The spin coating process is strongly dependent on the solvent and the interaction between solvent and surface. Therefore, a process can only be developed for a specific surface on which the monolayer should be based. With respect to the passivation concept presented in the subsequent section, a process for an Al$_2$O$_3$ and TOPCon (Tunnel Oxide Passivated Contact, [20,21,130,131], for further details see next section) surface is presented here. An extensive analysis about solvents and spin coating parameters on an Al$_2$O$_3$ surface can be found in my diploma thesis [127]. Within the present work, it was found that this process can be directly transferred to a TOPCon surface. The monodisperse SiO$_2$ spheres were transferred to a solution of 60% H$_2$O and 40% 2-propanol. This suspension was spin coated onto the Al$_2$O$_3$ or TOPCon surface by ramping up to 2000 rpm within 10 s and then switching to the final spin speed of 3250 rpm for 40 s. By this procedure, dense, hexagonally ordered monolayers (as depicted in Figure 59) are formed by self-organized growth.

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$^1$ Company: microparticles GmbH, Berlin
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Figure 59: SEM pictures of the SiO\(_2\) spheres after spin coating. A predominantly hexagonally ordered monolayer of spheres is visible. The pictures show a representative part of a 4-inch wafer.

Deposition of high refractive index material into the voids

In order to reach a high refractive index contrast and thus high diffraction efficiencies, a material with a refractive index as high as possible has to be used for the infiltration of the voids – in the following called inversion. Two options have been realized: TiO\(_2\) inversion using atomic layer deposition (ALD) and inversion using polycrystalline silicon (poly-Si) deposited by atmospheric pressure chemical vapor deposition (APCVD). The TiO\(_2\) deposition took place at 130° C and was done in a batch reactor at Beneq. The refractive index of the TiO\(_2\) is 2.38 for a wavelength of 1000 nm, compared to the refractive index of the spheres of 1.5, as determined by spectral ellipsometry [57]. Figure 60 (a) shows cross section SEM pictures after inversion.

The APCVD inversion with poly-Si took place at approximately 850° C. The refractive index contrast from silicon (3.55 at 1000 nm) to the spheres (1.5) is significantly higher for the APCVD-Si case. The deposited poly-Si can be doped by adding PH\(_3\) to the gas flow, which is important for contact formation. Both inversion methods lead to a structured surface; regularly and sphere-shaped for the TiO\(_2\) inversion, and stochastically and rough for the poly-Si inversion.

Figure 60: SEM pictures of the SiO\(_2\) sphere grating after inversion with TiO\(_2\) (a) or polycrystalline silicon (b). The voids in between the spheres are filled. The conformal growth of ALD leads to a regular, sphere-shaped surface, the poly-crystalline growth of APCVD leads to a stochastically rough surface.
Passivation concept

The spin coating processes described before have been developed for Al₂O₃ and TOPCon surfaces. The use of these surfaces is based on the goal to realize solar cells according to the EPOS concept (electrically planar, optically structured). Both, Al₂O₃ and TOPCon, can effectively passivate the rear surface of a silicon solar cell already with very low layer thicknesses (typically 10 nm for Al₂O₃ and about 20 nm for TOPCon). The additional optical structure therefore does not increase the recombination velocity while the very thin electrical passivation layer does not significantly influence the diffraction properties of the sphere grating. In order to reach high voltages and to avoid any voltage loss due to the additional optical structure, it has to be ensured that the process steps for the grating fabrication do not deteriorate the passivation quality. The spin coating process itself influences neither the Al₂O₃ surface nor the TOPCon surface. The more critical process is the void infiltration as it takes place at higher temperatures. In reference [127] it was shown, that in the case of TiO₂ ALD the passivation quality of a 10 nm thick Al₂O₃ layer is not deteriorated. More important for the realization on final device level within this work is the combination of the APCVD infiltration of poly-Si with the TOPCon surface. In test batches a process sequence has been developed that allows for a passivation quality after the complete fabrication that is equally high than without the sphere grating processes. The TOPCon process itself comprises an oxidation for the tunnel oxide, the deposition of a semi-crystalline Si-rich layer, a temperature annealing at 800 °C and an hydrogen based annealing step at 400 °C [20,21,130,131]. To investigate the influence of the APCVD inversion process on the passivation quality, symmetrical life time samples with TOPCon on both sides have been processed on float zone silicon wafers with 1 Ωcm. After TOPCon passivation, they feature initial life time values of above 2.5 ms corresponding to implied open circuit voltage (iV_Oc) values of approximately 720 mV. After both grating fabrication steps (spin coating and APCVD deposition at 850 °C, grating only on one side of the wafer), the passivation quality significantly decreased as can be seen in Figure 61. This effect can be attributed to the high temperature of the APCVD process, because at this temperature the hydrogen content of the TOPCon layer is reduced and thus the passivation quality. A subsequent hydrogen annealing step was therefore applied and a full recovery of the passivation quality was reached. This hydrogen annealing step is identical to the one usually used for the TOPCon passivation except of a higher temperature of 450 °C that further accelerates the hydrogen diffusion through the APCVD poly-Si layer to the TOPCon interface. After this annealing, which can replace the first hydrogen annealing step, iV_Oc-values in the range of 720 mV were obtained. This shows that with respect to the passivation, the TOPCon interface is fully compatible with the sphere grating fabrication. [128]
Figure 61: Life time and $iV_{OC}$ results obtained from minority carrier life time measurements (QSSPC) of symmetrical life time samples with TOPCon on both sides. The sphere grating processes significantly reduce the passivation quality, but with an additional hydrogen annealing step, the initial values can be fully recovered.

**Contact formation**

The two infiltration processes (ALD, APCVD) have a further important difference: While the TiO$_2$ deposited by ALD is not conductive, the silicon deposited via APCVD can be made conductive by adding doping gases (PH$_3$ for n-type) in the deposition process. In combination with the full area passivating contact TOPCon underneath, this allows for a full area passivating contact including the optical structure. In contrast, the TiO$_2$ matrix would require additional local contact openings. Furthermore, the silicon matrix allows for an even higher voltage level, due to the very good passivation properties of TOPCon. Therefore, within this work solar cells were processed following only the second approach (see 5.3.3).

Doping the poly-Si matrix with phosphorous also induces further parasitic absorption due to increased free carrier absorption (FCA). Thus the conductivity, which requires doping, has to be balanced with the parasitic absorption. In order to determine the doping level required for sufficient conductivity, various contact resistance samples were processed. There are several interfaces that have to be investigated with respect to their contact resistance: c-Si bulk to TOPCon, TOPCon to the poly-Si matrix, and the poly-Si matrix to the rear silver layer. For a PH$_3$ gas flow of 16 sccm in the APCVD chamber, contact resistance measurements of samples as depicted in Figure 62 yielded values in the range of 10 mΩcm$^2$, which is similar to the contact resistance for a TOPCon interface without sphere grating. A reduction of the gas flow to 12 or even 8 sccm led to significantly higher resistances. Therefore 16 sccm, which corresponds to a doping level of approximately $1e19$ cm$^{-3}$, was chosen for the processing of first solar cells.
Figure 62: Sample geometry for measuring the contact resistance through the complete rear side structure.

To further minimize the parasitic absorption due to FCA in the poly-Si, a reduction of the doping level by using a variable doping profile was investigated. Such variable doping profiles are in principle easy to realize, as the gas flow of PH$_3$ can be adjusted during the APCVD process. In addition to the samples as depicted in Figure 62, further samples with less layers at the rear have been fabricated in order to deduce contact resistances of individual interfaces. The measurements altogether indicated that the contact resistances of TOPCon to the poly-Si and from poly-Si to silver are the most critical ones. The conductivity of the poly-Si itself is not limiting the contact resistance when the doping level is reduced. Thus, for the solar cells presented in 5.3.3, the two types of doping profiles depicted in Figure 63 have been tested. For optical reasons (to avoid parasitic absorption in the metal), an additional ITO layer was deposited in between the poly-Si matrix and the silver. In pretests, the introduction of this additional ITO layer did not significantly change the contact resistance of the complete structure.

Figure 63: Two different doping profiles of the poly-Si matrix deposited by APCVD. On the left side a constantly high doping that allows for a low contact resistance of the complete rear side in the range of 10 mΩcm$^2$. On the right side, only the interfaces to TOPCon and to ITO have been highly doped, while the largest part of the poly-Si matrix features a lower doping level that still allows for a large enough conductivity.

5.3.2 Optical characterization of sphere gratings

The measured absorptance enhancement of samples with TiO$_2$-inverted sphere gratings is mentioned briefly in the next section before the samples with poly-Si are investigated in detail in the subsequent section. Due to the superior passivation quality of TOPCon and the possibility to realize a full area
contact at the rear, the sphere gratings inverted with poly-Si deposited by APCVD were in the focus of this work and of the following optical characterization.

**Samples with TiO$_2$ inversion**

The absorption for the sample depicted in Figure 60 (a) was determined by a center mount measurement in an integrating sphere using a Cary 5000i. By such a “center mount” measurement setup all light that is not absorbed inside the sample is detected. To determine just the absorption enhancement in the silicon bulk, a metal rear reflector, which would be necessary in complete solar cells, has not been deposited. Several simulations verified that for systems without a mirror a very similar absorption enhancement can be expected as for systems with a mirror. Only small changes or spectral shifts of the absorption enhancement have been observed in the outcome of the simulation. Thus the measurements can be seen as a strong evidence for the light trapping properties of fully processed solar cells. The measurements presented in Figure 64 show a significant absorption enhancement in the near infrared due to the sphere grating corresponding to a photocurrent density gain of 1.04 mA/cm$^2$ and 1.49 mA/cm$^2$ for a wafer thickness of 250 µm and 100 µm, respectively. Due to the absorption enhancement, the photocurrent density in a wafer with a thickness of 100 µm with the sphere grating exceeds the photocurrent density in a planar wafer with a thickness of 250 µm. This highlights the potential of the proposed light trapping concept with regard to thinner solar cells. [57]

![Absorption measurement graphs](image)

Figure 64: The left graph shows the results of the absorption measurements of wafers with a planar front and a TiO$_2$-inverted sphere grating at the rear in comparison to flat reference wafers. The absorption enhancement (difference between samples with grating and flat reference) is shown on the right. For thinner wafers, the maximum absorption enhancement occurs for shorter wavelengths, as expected from theory. [57]

**Samples with silicon inversion**

For the optical investigation of sphere gratings inverted with poly-Si, different samples have been prepared. Table 7 gives an overview of the processed samples. In order to determine the absorption enhancement due to the sphere grating, hemispherical reflectance measurements have been conducted using an integrating sphere in a Cary 5000i. To approach the situation in the final solar cell configuration, a high-quality silver mirror was attached behind the samples. The remaining air gap between the sample and the mirror in combination with the mirror itself leads to a very high rear side reflectance with very low parasitic absorption. Thus, these optical measurements can be seen as an
5 Experimental realization of light trapping structures

upper limit for the beneficial effect of the grating in fully processed solar cells including an additional mirror at the rear.

Table 7: Samples processed for optical characterization.

<table>
<thead>
<tr>
<th>Textures front/rear</th>
<th>Cell thickness [µm]</th>
<th>Detailed structure at the rear</th>
</tr>
</thead>
<tbody>
<tr>
<td>Planar/planar</td>
<td>200</td>
<td>planar</td>
</tr>
<tr>
<td>Planar/sphere grating</td>
<td>200</td>
<td>TOPCon + spheres with poly-Si thickness of 1 µm</td>
</tr>
<tr>
<td>Random pyramids/planar</td>
<td>200</td>
<td>planar</td>
</tr>
<tr>
<td>Random pyramids/sphere grating</td>
<td>200</td>
<td>TOPCon + spheres with poly-Si thickness of 1 µm</td>
</tr>
</tbody>
</table>

Figure 65: Absorptance (calculated via 1-R from measurements) for a planar or textured (random pyramids) front surface combined with a planar or sphere grating rear side. An external Ag mirror was placed behind the sample. The sphere grating leads to a significant absorption enhancement, for both front surfaces, resulting in an absorptance close to the Lambertian limit (calculated). [128]

Figure 65 shows the measurement results for all sample types. A clear absorptance enhancement due to the sphere grating is visible in the NIR. For samples with planar front surface, the enhancement corresponds to a possible photo current density gain of 1.6 mA/cm². For samples with textured front, the gain is much smaller, as the front texture already leads to a light path length enhancement. Nevertheless, the sphere grating increases the absorption further by 0.4 mA/cm². For both cases also the case of a perfectly Lambertian scatterer at the rear (calculated according to eq. (16)) is added to Figure 65 demonstrating that the sphere grating leads to light trapping close to the Lambertian limit. It is important to keep in mind that such an optical measurement does not allow for an accurate determination of the current density gain, as it is impossible to distinguish between useful absorption in the silicon bulk and parasitic absorption. By using the external mirror, the parasitic absorption was kept low, but still the grating itself, especially the doped poly-Si matrix, features parasitic absorption. In order to separate these effects, results on solar cell level are presented in the section 5.3.3.
Parasitic absorption in samples with sphere grating at the rear

Two major origins of parasitic absorption have been identified: the plasmonic absorption in the rear side metal (especially when it is structured) and the parasitic absorption (FCA) in the poly-Si matrix. To reduce the parasitic absorption in the metal layer, a wet-chemical process that flattens the rear after the poly-Si deposition was developed. Using an etching solution consisting of HF, HNO\(_3\), H\(_2\)SO\(_4\) and H\(_2\)O allows for a considerable flattening of the rough poly-Si surface. Figure 66 shows the poly-Si surface as-deposited (left) and after the flattening (middle). A further option to reduce parasitic absorption in the metal is a dielectric buffer layer between poly-Si and Ag. On the right side of Figure 66 the poly-Si surface is shown after spin coating of a SiO\(_2\) nanoparticle solution. The spin coating leads to a significantly smoother surface compared to the as-deposited surface and also the Ag layer is shielded.

Figure 66: SEM pictures of the APCVD-Si surface after deposition (left), after wet chemical etch back (middle) and after the deposition of a planarizing solgel layer of SiO\(_2\) (right).

Both flattening strategies have been investigated with respect to their influence on the parasitic absorption. Therefore, further sample types (given in Table 8) have been processed and characterized via photospectrometry.

Table 8: Sample types for optical characterization of parasitic absorption in the rear side metal.

<table>
<thead>
<tr>
<th>Textures front/rear</th>
<th>Cell thickness [µm]</th>
<th>Detailed rear side structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Random pyramids/sphere grating</td>
<td>200</td>
<td>TOPCon + spheres with poly-Si thickness of originally 5 µm, then etched back, then deposition of Ag (sample type 1)</td>
</tr>
<tr>
<td>Random pyramids/sphere grating</td>
<td>200</td>
<td>TOPCon + spheres with poly-Si thickness of originally 5 µm, then etched back, then deposition of SiO(_2) buffer layer, then Ag deposition (sample type 2)</td>
</tr>
<tr>
<td>Random pyramids/sphere grating</td>
<td>200</td>
<td>TOPCon + spheres with poly-Si thickness of 5 µm, then deposition of Ag (sample type 3)</td>
</tr>
<tr>
<td>Random pyramids/sphere grating</td>
<td>200</td>
<td>TOPCon + spheres with poly-Si thickness of 5 µm, external high-quality mirror behind (sample type 4)</td>
</tr>
</tbody>
</table>
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The results presented in Figure 67 show that it is crucial to use a buffer layer in between the sphere grating and the Ag layer. Reducing a part of the roughness by wet chemical etching alone is not sufficient for reducing the parasitic absorption. Using a smoothing spacer layer leads to an absorption similar to the one with detached high-quality silver mirror. SiO₂, which has been tested as buffer layer here is not conductive and would require an additional local contact opening. Therefore, for the solar cells, ITO has been used as buffer layer. While the refractive index of ITO is slightly higher it allows for a full area rear side contact as targeted.

Figure 67: Absorption measurement of samples with different rear reflectors behind the sphere grating. A detached Ag mirror leads to the lowest parasitic absorption at 1200 nm, an evaporated Ag layer with a SiO₂ buffer layer also strongly reduces the parasitic absorption. The wet chemically flattened rear with a directly evaporated Ag mirror cannot significantly reduce the parasitic absorption.

The second parasitic absorption mechanism is FCA in the doped poly-Si. To get a qualitative impression of the amount of parasitic absorption in the poly-Si layers, Figure 68 shows the absorptance curves of two samples with sphere grating: one with an undoped poly-Si matrix and one with a doped poly-Si matrix. Both APCVD layers feature a thickness of 5 µm. For the doped samples, a gas flow of 16 sccm PH₃, corresponding to the value needed for sufficiently low contact resistances, was used. An external, high-quality silver mirror was used behind the sphere grating in order to minimize parasitic losses that are not related to the doping of the poly-Si. Figure 68 shows that in order to minimize parasitic absorption it is crucial to keep the doping within the poly-Si matrix and its thickness as low as possible.
The optical investigation of parasitic absorption can serve only as a rough estimation for the actual parasitic absorption. However, two guidelines for the processing of complete solar cells have been deduced: First, a buffer layer is necessary and second, the thickness and the doping level of the poly-Si matrix have to be kept as low as possible, which again explains the approach presented in Figure 63.

### 5.3.3 Solar cells with sphere gratings at the rear

With regard to the characterization results of minority carrier life time, contact resistance and optical absorbance enhancement, a first batch of solar cells with a structure as depicted in Figure 69 was fabricated. Similar to the binary grating cells, 7 cells (2x2cm²) were processed on each four inch wafer (shiny-etched, 1Ωcm, (100)-oriented n-type FZ Si). The thickness of the wafers was 200 µm and thus slightly thinner than for the cells with binary gratings. The TOPCon (Tunnel Oxide Passivated Contact) has been realized according to [130,132]. An implanted boron doped p-type emitter with a sheet resistance of 150 Ω/sq. and a boron doped diffused selective emitter with 9 Ω/sq. underneath the metal contacts were fabricated. The emitter has been passivated with 10 nm ALD-deposited Al₂O₃. The front grid was defined via photolithography and seed layers consisting of a stack of Ti, Pd, and Ag were evaporated. By light induced plating the grid lines were thickened.
5.3.3.1 First solar cell batch with sphere gratings

For the first solar cells fabricated with sphere gratings, a double layer antireflection coating consisting of PECVD-deposited SiN$_x$ and evaporated MgF$_2$ was applied to a planar front surface and the poly-Si sphere grating matrix was doped with phosphorus to a level of approximately $1 \times 10^{19}$ cm$^{-3}$ (PH$_3$ flow 16 sccm). The deposited matrix had a thickness of 5 µm and was etched back with a planarizing wet-chemical process (etching solution based on HF, HNO$_3$, H$_2$SO$_4$ and H$_2$O). For further planarization and contact formation a 150 nm thick ITO layer was deposited by sputtering followed by thermal evaporation of silver. These first solar cells with sphere gratings were added to a solar cell batch that was originally planned for basic investigations regarding TOPCon. For this purpose, usually solar cells with a textured front are used, and thus, no reference solar cells without sphere gratings with a flat front surface have been fabricated and the total number of cells with sphere grating was very small. The results presented in Table 9 demonstrate the successful integration of sphere gratings into fully processed solar cells. $V_{OC}$ and $FF$ are very high and close to the values reported for TOPCon solar cells without sphere gratings. The excellent passivation, the very good fill factor and the remarkably high short circuit current density for a solar cell with planar front lead to an overall efficiency of the best cell of 22.1%. This is significantly higher than the efficiency of the best NIL grating cell with planar front and grating rear (19.0%, section 5.2.3), mainly due to two reasons: the higher voltage level due to TOPCon and the higher current due to a significantly better ARC. To evaluate and compare the optical effect of the sphere grating, EQE measurements have been performed.

Table 9: Solar cell parameters from light $IV$-measurements for solar cells with planar front and sphere grating at the rear. The result for the best cell has been independently confirmed by Fraunhofer ISE CalLab. For the average cells, a usual $IV$-measurement has been conducted using the best cell as calibration cell. [128]

<table>
<thead>
<tr>
<th></th>
<th>$V_{OC}$ [mV]</th>
<th>$J_{SC}$ [mA/cm$^2$]</th>
<th>$FF$ [%]</th>
<th>$\eta$ [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average (6 cells)</td>
<td>703±5</td>
<td>38.0±0.1</td>
<td>80±3</td>
<td>21.3±0.9</td>
</tr>
<tr>
<td>Best cell*</td>
<td>710</td>
<td>38.1</td>
<td>81.9</td>
<td>22.1</td>
</tr>
</tbody>
</table>

*confirmed by Fraunhofer ISE-CalLab
As no flat reference cells were available, Figure 70 shows the EQE measurement of the best solar cell with sphere grating and in comparison a simulated EQE of a both side planar reference cell. Note that for the planar reference (black curve), an absorption curve has been simulated with a lossless flat mirror at the rear. This gives an upper limit for a planar-planar solar cell with the same ARC. A significant EQE enhancement in the NIR, corresponding to a $J_{SC}$ gain of 1.4 mA/cm² (meaning an efficiency gain of 0.8 % absolute), is observed and displayed by the dashed orange curve. This qualitatively confirms the results of the optical investigations presented in section 5.3.2, but quantitatively the gain demonstrated with solar cells is slightly lower than for the optical samples, especially considering that the optical samples featured no antireflection coating at all. This indicates parasitic absorption in the rear structure as discussed in section 5.3.2.

Figure 70: EQE curve for a solar cell with a planar front and a sphere grating at the rear (orange line). In comparison, the absorption in a planar-planar wafer with a lossless flat rear side mirror (black line) is significantly lower. The EQE gain, shown by the dashed orange line, corresponds to a photocurrent density increase of 1.4 mA/cm². [128]

Figure 71 shows SEM pictures of the cross section of solar cells with fully processed rear surface. The pictures show a structure as desired and sketched in Figure 63. The additional APCVD layer thickness on top of the spheres varies approximately between 1 and 2 µm due to inhomogeneities of the APCVD process. The gap visible between the ITO layer and the silver layer is related to the preparation of the cross sections.
Figure 71: SEM cross section of the sphere grating at the rear of a silicon solar cell. The two pictures show two different spots on the same wafer. The c-Si bulk layer can be seen at the bottom, the TOPCon layer is too thin to be visible. The poly-Si fully infiltrated the voids in between the spheres and covers the sphere layer with an additional layer thickness that varies between less than 1 µm (left picture) and about 2 µm (right picture). On top, the ITO and silver layer complete the rear contact.

5.3.3.2 Second solar cell batch with sphere gratings

As already discussed in the previous section, parasitic absorption is an important issue for the sphere grating cells. In a second solar cell batch, the solar cell concept of the first cells was realized with a larger number of cells including references with both, planar and textured front surface, and additionally sphere grating cells with a gradient doping profile like presented in Figure 63. However, the MgF₂ deposition, which is the last step at all, was very inhomogeneous and led to a significantly too large MgF₂ thickness. Therefore all following results are based on measurements that have been conducted before the erroneous MgF₂ deposition just with a single layer SiNₓ ARC with a thickness optimized for the use in a double layer ARC. Hence, the overall level of efficiency is slightly lower than in the first batch.

Cells with planar front surface

Table 10 summarizes the best solar cell’s results for each group before MgF₂ deposition and shows that also in this batch, highly efficient solar cells including sphere gratings have been successfully fabricated. Despite the larger number of cells within this solar cell batch, one should still be very careful with drawing conclusions from single parameters like in Table 10.

Table 10: Solar cell parameters from light IV-measurements for solar cells with planar front and sphere grating at the rear. Two different doping profiles in the sphere grating matrix (high and high-low-high as presented in Figure 63) have been compared.

<table>
<thead>
<tr>
<th>Front</th>
<th>Best Cells</th>
<th>Rear</th>
<th>$V_{OC}$ [mV]</th>
<th>$J_{SC}$ [mA/cm²]</th>
<th>FF [%]</th>
<th>η [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Planar</td>
<td>Planar</td>
<td>Planar</td>
<td>720</td>
<td>36.3</td>
<td>82.7</td>
<td>21.7</td>
</tr>
<tr>
<td>Planar</td>
<td>Spheres (high)</td>
<td></td>
<td>715</td>
<td>37.2</td>
<td>81.8</td>
<td>21.8</td>
</tr>
<tr>
<td>Planar</td>
<td>Spheres (high-low-high)</td>
<td></td>
<td>714</td>
<td>37.8</td>
<td>81.0</td>
<td>21.8</td>
</tr>
</tbody>
</table>
For a better description of the variations and a graphical impression of trends, Figure 72 shows all measured cell parameters for the three different groups (reference, high, high-low-high doped matrix). It can be seen that on average 10-15 mV are lost in $V_{OC}$ for the cells including sphere gratings independent of the doping profile. Also the average fill factor is slightly reduced for the sphere grating cells. The short circuit current density is significantly enhanced, similar to the results based on the optical results and the first batch. Both effects roughly compensate each other leading to a similar efficiency level for reference and sphere grating cells.

![Graph showing measured Jsc, Voc, FF and efficiency η of crystalline silicon solar cells with planar front surface and planar (pp) or sphere grating rear side (pg) and different doping profiles in the sphere grating. Crosses show the result for all individual cells, the boxplots show median and 25/75 percentile.](image)

Figure 72: Measured $J_{SC}$, $V_{OC}$, $FF$ and efficiency $\eta$ of crystalline silicon solar cells with planar front surface and planar (pp) or sphere grating rear side (pg) and different doping profiles in the sphere grating. Crosses show the result for all individual cells, the boxplots show median and 25/75 percentile.

In order to investigate the beneficial effect of the sphere grating to the short circuit current density and especially the effect of the gradient doping profile (high-low-high) in comparison to the highly doped poly-Si matrix also used in the first sphere grating batch, EQE measurements have been conducted. Figure 73 shows EQE curves for the three different groups of cells. Similar to the results presented in Figure 70, the sphere grating with a constant doping profile leads to a significant EQE enhancement corresponding to a photo current density gain of 1.1 mA/cm$^2$ in the NIR between 1000 and 1200 nm. Note that the values are not directly comparable to the results of the first batch due to the different ARCs at the front. The gradient doping profile leads to an even higher EQE corresponding to a photo
current density gain of 1.4 mA/cm². This indicates the reduction of parasitic absorption (free carrier absorption), which was the objective of using this doping profile.

Figure 73: EQE measurements of cells with planar front and different rear structures. The planar TOPCon-silver reference in black, two cells with sphere gratings featuring a constant doping profile (high) in green and orange and two cells with a high-low-high doping profile in light green and blue.

**Cells with textured front**

In this second batch, also sphere grating and reference cells with textured front were included. Table 11 shows the best cell’s parameters, which have again to be interpreted with caution. Figure 74 summarizes the parameters of all measured cells. The reduction in voltage and fill factor induced by the sphere grating is slightly larger than for the cells with planar front. No short circuit current density enhancement by the grating can be seen. On the contrary, the sphere grating seems to reduce the $J_{SC}$ leading to an overall significantly lower efficiency for the sphere grating cells.

Table 11: Solar cell parameters from light $IV$-measurements for solar cells with textured front and sphere grating at the rear. Two different doping profiles in the sphere grating matrix (high and high-low-high as presented in Figure 63) have been compared.

<table>
<thead>
<tr>
<th>Front</th>
<th>Best Cells</th>
<th>Rear</th>
<th>$V_{OC}$ [mV]</th>
<th>$J_{SC}$ [mA/cm²]</th>
<th>FF [%]</th>
<th>η [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Textured</td>
<td></td>
<td>Planar</td>
<td>722</td>
<td>40.9</td>
<td>82.0</td>
<td>24.2</td>
</tr>
<tr>
<td>Textured</td>
<td></td>
<td>Spheres (high)</td>
<td>712</td>
<td>40.7</td>
<td>80.3</td>
<td>23.3</td>
</tr>
<tr>
<td>Textured</td>
<td></td>
<td>Spheres (high-low-high)</td>
<td>716</td>
<td>40.2</td>
<td>79.0</td>
<td>22.8</td>
</tr>
</tbody>
</table>
Experimental realization of light trapping structures

Figure 74: Measured $J_{SC}$, $V_{OC}$, $FF$ and efficiency $\eta$ of crystalline silicon solar cells with random pyramids at the front surface and planar (tp) or sphere grating rear side (tg) and different doping profiles in the sphere grating. Crosses show the result for all individual cells, the boxplots show median and 25/75 percentile.

To understand the effect of the sphere grating in more detail, Figure 75 shows EQE measurements of the best solar cell of each group. The constantly high doping of the sphere grating matrix leads to a decreased EQE in the NIR compared to the textured-planar reference solar cell. For the high-low-high doping profile the EQE is higher than for the constantly high doping profile, which indicates a reduction of parasitic absorption as already seen for cells with planar front surface. However, the EQE is still not higher than the one of the reference solar cell. Thus, the gradient doping can reduce the parasitic absorption, but parasitic effects still compensate any beneficial light trapping effect of the grating. Note that the difference in Figure 75 at 800 nm is related to variations at the front (variation of ARC and/or metallization) and not to the grating.
Figure 75: EQE measurements of cells with textured front and different structures at the rear. The planar TOPCon-silver reference in black, a sphere grating cell featuring a constant doping profile (high) in green and a cell with a high-low-high doping profile in orange.

To summarize, the sphere grating in this solar cell concept is not beneficial to solar cells with a front surface textured with random pyramids, while a significant gain has been demonstrated for solar cells with planar front. The light trapping in the reference cells with textured front and planar rear is already on a high level and a small light path length enhancement due to the sphere grating indicated by optical measurements is overcompensated by parasitic absorption losses and the slight decrease of voltage and fill factor due to the sphere grating processes.

5.3.4 Comparison to simulations

Within this section, OPTOS simulations are compared with the previously described measurements. Besides the basic physical understanding and validation, the purpose of such a comparison is the identification of possible loss mechanisms and options for a further optimization of the fabricated structures. To run an OPTOS calculation corresponding to the fabricated solar cells, redistribution matrices for the front and rear surfaces are needed. The front surface is either planar or textured with random upright pyramids, in both cases featuring additional ARC layers. The following simulations focus mainly on the solar cells with planar front surface, because in this case all matrices used in OPTOS can be simplified with regard to the angular discretization. In a system with a planar front and a grating rear, only a finite set of diffraction orders appears for normal incidence. In all subsequent interactions between front and rear surface, this finite set remains unchanged, as the grating redistributes light only between these diffraction orders, and the planar front causes only specular reflection, as described in [54] and in section 3.2.1. This allows for an enormous reduction of the number of computationally demanding RCWA calculations needed for a sphere grating matrix. In the following a short description of the calculation of such sphere grating matrices is given.
Implementation of the sphere grating in RCWA code RETICOLO 2D

The sphere grating consists of a hexagonally ordered monolayer of spheres with a diameter of 966 nm. The code RETICOLO 2D [76,77] requires a rectangular unit cell, which leads to a unit cell as depicted in Figure 76 (a). This unit cell has the double area of an elementary hexagonal unit cell. Furthermore, the method requires a segmentation of the grating structure into a stack of planar layers (Figure 76 (b)) and an approximation of the circular cross sections of the spheres within each of these planar layers by rectangles as depicted in Figure 76 (c). It is important to consider enough Fourier orders (especially more Fourier orders in y-direction than in x-direction), enough rectangles to approximate a circle and enough thin planar layers to build up a sphere. Detailed convergence analyses for these parameters can be found in [127]. Within this work, at least two more Fourier orders were considered than propagating orders in the far field exist for the specific combination of wavelength, grating period and refractive index. At least 50 layers in z-direction have been used to approximate a sphere and at least 15 rectangles to approximate a circular cross section.

Figure 76: (a) shows the rectangular unit cell used for a hexagonal grating. The aspect ratio of the unit cell is \( \sqrt{3} \). (b) shows the discretization in z-direction (8 layers used in this sketch to create a sphere). (c) shows that the circular cross sections are approximated by a number of rectangles (three in this simplified sketch). Based on [127].

Creation of redistribution matrices based on the RCWA results

In contrast to all matrices presented so far within this work, sphere grating matrices cannot be fully described by a symmetry element that is restricted to azimuth angles between 0 and 45° as presented in Figure 12. Due to the choice of the unit cell depicted in Figure 76 (a), also the 60°-symmetry of the hexagonal grating cannot be utilized. Instead, azimuth angles between 0 and 90° have to be considered. For all larger angles between 90 and 360° a symmetrically corresponding angle between 0 and 90° can be assigned. Therefore all sphere grating matrices feature azimuth angles from 0 to 90°, which means that also matrices for the front that are to be combined with sphere grating matrices have to contain these angles.

For a complete matrix corresponding to a rear as shown in Figure 71, a fully coherent result would strongly depend on the exact additional layer thickness of the poly-Si, while this layer thickness varies at least between 1 µm and 2 µm. Possible coherent coupling effects between the sphere grating and the
ITO-Ag rear are averaged out by the strongly varying poly-Si thickness and further reduced by the surface roughness of the poly-Si. Therefore, an incoherent approach similar to the one used for binary grating matrices has been chosen. Such an incoherent coupling of the sphere grating with the ITO-Ag mirror is assumed to be the most realistic description of the real samples. The approach is summarized in Figure 77.

Figure 77: Approach for the calculation of sphere grating matrices. A matrix for the sphere grating and a matrix for the Si-ITO-Ag interface are combined incoherently and for the final calculation the resulting effective redistribution matrix is used.

As the APCVD-Si is crystalline, the refractive index data by Green [10] have been used. Additional parasitic absorption (e.g. FCA) can be accounted for by enhancing the imaginary part of the refractive index $k$, for example considering equations (21) and (22).

Using such effective sphere grating matrices in combination with planar front matrices adapted to the SARC layer thickness of the solar cells, the absorptance within the silicon bulk has been calculated. To account for the metal front grid, which is not considered in the calculation of the matrix corresponding to the front, the simulated absorptance curve has been corrected by -3% rel. Figure 78 shows that for the planar reference cells, simulation and measurement are in very good accordance. The good agreement of simulation and measurement in the short wavelength range indicates a correct description of the solar cell’s front surface. For the cells with sphere grating at the rear, however, the OPTOS simulations yield a higher absorption gain in the near infrared when sphere grating matrices without additional parasitic absorption are used. As already indicated by measurements and described in section 5.3.1, parasitic absorption in the rear structure probably reduces the gain due to the grating. The parasitic absorption can have several sources, especially free carrier absorption (FCA) in the doped poly-Si, defect state absorption in the poly-Si and enhanced parasitic absorption in the silver due to a structured interface. FCA in the poly-Si can be accounted for by adapting the imaginary part of the refractive index $k$ in the RCWA-based matrix creation. Assuming a $k$ according to equation (22), however, leads to a negligible amount of parasitic absorption and cannot explain the deviation. It remains questionable, if equations (21) and (22) reflect the correct parameterization of FCA in the deposited poly-crystalline silicon. This parameterization has been determined by Ruediger et al. using
float-zone silicon. Due to this uncertainty, also here an assumed additional loss of 10 and 20% for each interaction with the rear has been tested (as described for the binary gratings in section 5.2.4) to check the assumption that the deviation is caused by parasitic losses. This can be done by multiplying the effective sphere grating matrix with a factor of 0.9 or 0.8. Assuming 20% parasitic loss leads to a good agreement between the simulation and the solar cell from the first solar cell batch (section 5.3.3.1). To match the second solar cell batch, where parasitic losses were reduced by using a high-low-high doping profile, a loss of 10% has to be assumed. This indicates that the assumption of parasitic absorption is correct and that reducing these parasitic absorption losses would allow for even higher absorption gains. However, this approach cannot identify, where this parasitic absorption exactly occurs.

Figure 78: OPTOS calculations in comparison with EQE measurements for a 200 µm thick cell with planar front and planar or sphere grating at the rear. A factor of 0.9 for the effective sphere grating redistribution matrix (means 10 % losses at each interaction with the rear) accounts for a parasitic absorption loss at the rear side without exactly knowing its origin. It leads to a result similar to the measurement. The lower graph shows the simulated (including 10 % losses) and measured (high-low-high grating doping) EQE gain due to the grating for a planar front. Note that the drop in absorptance between 1110 and 1120 nm is related to the appearance of the diffraction order (3,1) for normal incident light (compare eq. (8)).

For solar cells with textured front, the experimental results showed no EQE gain due to the grating. In Figure 78, OPTOS simulation results are added to the measurement results and it is shown that the
sphere grating without additional parasitic absorption loss could lead to a significant absorptance enhancement. Weighted with the AM1.5g spectrum, the absorptance enhancement corresponds to a photo current density gain of 1.0 mA/cm$^2$. However, if the 10% parasitic loss is considered, which was needed to match the simulations for cells with planar front surface, the complete absorptance gain is compensated. The simulated absorptance curve with 10% loss at the rear structure is very similar to the simulated reference curve with planar rear – in accordance to the EQE measurements. This emphasizes that it would be crucial to reduce the parasitic losses in order to demonstrate the beneficial effect of the sphere grating also for solar cells with textured front. The OPTOS simulation result reveals that in principle, a significant gain due to a sphere grating for a solar cell textured at the front is possible.

Figure 79: OPTOS calculations in comparison with EQE measurements for a 200 µm thick cell with random pyramids front texture and planar or sphere grating rear side. A factor of 0.9 for the rear redistribution matrix (means 10% losses at each interaction with the rear) accounts for a parasitic absorption loss at the rear without exactly knowing its origin. It leads to a result similar to the measurement. The lower graph shows the simulated and measured EQE gain due to the grating.
6 Comparison and evaluation of different light trapping structures

On the background of the results presented in chapter 4 and 5, in this chapter various light trapping structures are compared and evaluated. The simulation formalism OPTOS is used to give an overview over achievable photo current densities for different texture combinations and different cell thicknesses. The experimentally realized grating structures are compared to each other, also using OPTOS to overcome the problem of different solar cell thicknesses used in the experiments. At the end of the chapter, I give a short outlook towards Si-based tandem solar cells, where diffractive gratings might be a promising approach.

6.1 Simulation based comparison of different texture combinations

So far, nearly all high-efficiency c-Si solar cells feature a pyramidal texture at the front surface and either a planar mirror or a further pyramidal texture at the rear. Within this section, I compare all structures presented in the previous two chapters, especially gratings, with state-of-the-art random pyramids with respect to the performance in the complete spectral range. Also solar cells with planar front are compared with respect to various light trapping structures at the rear.

As described in section 3.2, OPTOS is an efficient formalism to incoherently couple two or more textured interfaces. As the matrices, once calculated with the most suitable method, can be reused, a matrix database was established. In the following a fraction of these matrices is combined in different ways with varying cell thicknesses in order to demonstrate, which structures or structure combinations might be suitable for silicon solar cells. The results presented here were obtained in parallel to the experimental work presented in the previous chapter and strongly influenced the experimental realization, especially with regard to grating parameters, parasitic absorption in the metal and to the combination of front side textures and rear side gratings.

6.1.1 Solar cells with planar front surface

Figure 80 gives a first overview for cells with a planar front surface and different rear sides: a planar silver mirror, random pyramids with MgF$_2$ and silver as proposed by Holman et al. [133] and a perfect Lambertian scatterer. It is evident that for planar solar cells a very good front antireflection layer is absolutely necessary. By adding a structured rear side (here: Lambertian or random pyramids), the photo current density can be enhanced significantly. Random pyramids at the rear with a MgF$_2$/Ag
mirror leads to slightly lower values than a Lambertian scatterer. Additionally, the red line in Figure 80 shows the hypothetical photo current density for the case of zero front surface reflectance and a specular rear side mirror. In this case there is no light trapping at all within the solar cell and thus, it gives an upper limit for systems without light trapping. For thinner solar cells, where light trapping gets more and more important, such a system leads to lower photo current densities as systems with (non-ideal) front side ARCs and rear side light trapping structures.

Figure 80: Calculated photo current densities of solar cells with planar front surfaces (no ARC, SARC, DARC, perfect ARC) and different rear sides (planar, Lambertian, random pyramids) for different cell thicknesses. Figure 80 contains no solar cells with rear side gratings. Different rear side gratings, which were investigated in chapter 5.2 and 5.3, are added in Figure 81. For reasons of readability only the values for one planar front side (SARC) are shown. The binary grating\(^1\) and the sphere grating\(^2\) lead to a similar photo current density gain, close to the one of random pyramids. For the experimentally realized solar cells with gratings an additional loss factor of 10% at the rear side was necessary to match the measured EQE. For the binary grating the values including such a 10% loss at the rear side are also added in Figure 81. A grating with optimized depth and profile shape\(^3\) (optimization done by Tucher [65]) is shown to exceed the Lambertian rear side scatterer. This shows the very high potential of binary rear side gratings.

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1 Grating parameters: crossed grating with a period of 1 µm, consisting of round a-Si pillars in air with a diameter of 800 nm and a grating depth of 180 nm, incoherently combined with an Al-foil rear side reflector
2 Grating parameters: hexagonally ordered monolayer of SiO\(_2\) spheres (diameter 966 nm) embedded in Si, incoherently combined with a silver rear reflector on top of the Si.
3 Grating parameters: crossed grating with a period of 1 µm, consisting of round Si pillars in air with an area related fill factor of 0.5 and a grating depth of 220 nm, incoherently combined with a specular reflector (R = 1)
Comparison and evaluation of different light trapping structures

6.1.2 Solar cells with textured front surface

All rear side structures presented in the previous section 6.1.1, have also been combined with front surfaces textured with random pyramids. The random pyramids reduce the front reflection loss and lead to light trapping, also without an additional rear side structure. Note the different scale of the y-axis in Figure 82 and the overall higher photo current densities compared to the solar cells with planar front surface. Additional to the light trapping by the random pyramids themselves, the photo current density can be further enhanced by rear side structures. Again, a Lambertian scatterer allows for slightly higher currents than a rear side textured with random pyramids with MgF\textsubscript{2} and a silver mirror. Figure 83 shows results for only one front side (random pyramids with SARC), but additionally for grating rear sides. Like for the cells with planar front side, the binary and the sphere grating allow for a photo current density close to the one that is reached with the Lambertian rear reflector. In contrast to the cells with planar front side, the optimized binary grating leads to a similar photo current density than the standard binary grating. One has to keep in mind, however, that the optimization was done for the combination with a planar front surface, where diffraction orders in the loss cone can be specifically suppressed, which is not necessarily an optimization for a textured front. A further optimization for a textured front side might be possible but has not been conducted within this work.
6.2 Comparison of fabricated light trapping structures

Throughout the previous chapters, various concepts have been investigated to improve light trapping in high-efficiency c-Si solar cells. In this section, the different concepts are compared to each other,
especially the experimental results on solar cell level. Such comparisons are difficult, as different solar cell concepts, cell thicknesses or different front side ARCs have been used.

Figure 84 (a) shows a direct comparison between the gain that has been reached using a sphere grating rear side or a binary crossed grating. Both gains are very similar considering the spectral position and the height. However, as the solar cells featured different thicknesses (200 µm for the sphere grating cells and 100, 150, 250 µm for the binary grating cells) the results are not directly comparable. Furthermore, different front side ARCs have been used. As shown in 5.2.4 and 5.3.4, the results for both grating types were simulated with good accordance to the experimental results using OPTOS. Thus, OPTOS enables a more direct comparison, as it allows for changing the cell thickness and the front side ARC. Figure 84 (b) shows the absorptance gain simulated for a 200 µm thick cell for both grating types and a front side with a 70 nm SiN$_x$ ARC. The two grating types lead to a very similar absorption enhancement. Integrated with the AM1.5g spectrum both absorption enhancements correspond to a current density gain of 1.4 mA/cm$^2$. For simple white paint or TiO$_2$ particles added externally to the rear side of an initially bifacial solar cell, a gain of 0.8 or 0.7 mA/cm$^2$ was reached compared to a silver mirror at the rear side (see Table 4). This gain was measured for solar cells with a double layer ARC. Thus it can be concluded that the diffractive structures developed within this work allow for a short circuit current density gain twice as high as simple diffuse rear side scatterers that are applied externally to a fully processed solar cell. The choice between sphere grating and binary grating can be made with respect to the solar cell concept and the process technology, the optical performance is very similar.

![Figure 84](image_url)

Figure 84: (a) Comparison of the EQE gains due to a sphere grating or a binary crossed grating compared to a flat mirror at the rear side. In addition to the different cell thickness, different front side ARCs have been used. While the cells with sphere grating featured a SiN$_x$ ARC, the binary grating cells featured a SiO$_2$ ARC. Sphere grating curve from Figure 78 and binary grating curves from Figure 55. (b) Using OPTOS, both grating types have been simulated in combination with a 70 nm SiN$_x$ front side ARC and a uniform cell thickness of 200 µm.

### 6.3 Outlook: Si-based tandem solar cells

To overcome the fundamental efficiency limits of a single junction silicon solar cell [3,4], Si-based tandem solar cells are of great interest. While a top cell made of a material with a higher bandgap...
allows for a better utilization of short wavelength photons, the silicon bottom cell absorbs the long wavelength photons. Therefore, a good near infrared light trapping is especially important for a silicon bottom cell. For many Si-based tandem solar cell concepts also a planar front side of the Si-bottom cell is required. This may be the case for perovskite on silicon [134] and also for III/V-cells on silicon, when wafer bonding or epitaxial growth is involved [135,136]. If a planar front surface is required, rear side structures like the gratings presented in section 5.2 and 5.3 are promising candidates for reaching efficient light trapping. Therefore, the presented solar cells with planar front and grating rear side could be a suitable bottom cell for tandem devices. The following section is based on [128] and demonstrates the efficiency potential of tandem devices (using real data) with a silicon bottom cell with a sphere grating rear side. Therefore, the EQE curve from the best sphere grating cell presented in 5.2.3 is combined with EQE curves for top cells taken from literature.

### 6.3.1 Perovskite on Silicon

For a perovskite-silicon tandem device, I used the published EQE-data for a single junction perovskite cell from Jeon et al. [137]. The EQE curves are displayed in Figure 85.

**Figure 85: EQE of the two solar cells used for the estimation of the performance of the perovskite-silicon tandem. For the silicon bottom cell two cases have been considered: for the black line, an estimate of the parasitic losses due to reflection and parasitic absorption in the top cell was considered; for the dashed line, a more idealized case with no such losses was considered in the spectral region above 600 nm. [128]**

Assuming an interconnection of both cells in a two-terminal device one can calculate an upper limit for the current density that is generated in the sub cells using the AM 1.5g photon number spectrum $N_{\text{AM15g}}$ and the elementary charge $q$ [128]:

$$J_{SC,\text{top}} = q \cdot \int_{0}^{800} \text{EQE}_{\text{top}} \cdot N_{\text{AM15g}} \, d\lambda$$

$$J_{SC,\text{bottom}} = q \cdot \int_{800}^{1200} (\text{EQE}_{\text{top,max}} - \text{EQE}_{\text{top}}) \cdot \text{EQE}_{\text{bottom}} \cdot N_{\text{AM15g}} \, d\lambda$$

(65)  

(66)
\[ J_{SC\text{,bottom high Transmission}} = q \cdot \int \frac{1200}{600} (1 - \text{EQE}_{\text{top}}) \cdot \text{EQE}_{\text{bottom}} \cdot N_{\text{AM1.5g}} d\lambda \] (67)

For the top cell, the integration spans the complete active region of the perovskite solar cell from 280 to 800 nm. For the bottom solar cell, the assumption is that all light with a wavelength shorter than 600 nm is either utilized in the top cell, or lost due to parasitic absorption and reflection. For wavelengths longer than 600 nm, two different cases for the transmission of photons through the top cell, represented by the equations (66) and (67), respectively, are considered. Case 1 assumes that the parasitic losses in the top cell (parasitic absorption and reflection), which limit the maximum value of the EQE of the Perovskite cell to \( \text{EQE}_{\text{top, max}} = 0.903 \), affect the whole spectrum. Furthermore, it is assumed that the EQE drop of the perovskite top cell in the wavelength range between 600 and 800 nm is attributed to transmission losses, which can be utilized by the bottom cell. The transmission losses at a certain wavelength are given by the difference of the highest EQE of the perovskite cell (\( \text{EQE}_{\text{top, max}} = 0.903 \)) and the EQE of the perovskite solar cell at the wavelength under consideration (see Eq. 66). This limits the EQE of the bottom cell to the values indicated in Figure 85 by the green area and the black line. In case 2, it is assumed that for wavelengths larger than 600 nm no parasitic losses in the Perovskite cell occur. Thus the transmission through the top cell is given by \( (1 - \text{EQE}_{\text{top}}) \), all light that is not used by the top cell is transmitted to the bottom cell (see Eq. 3). This is a more ideal case that would correspond to a top cell optimized for low reflectance and low parasitic absorption in the wavelength range above 600 nm. The resulting EQE is indicated by the dashed line and the lighter green area in Figure 85. Both calculations assume a perfect interconnection without optical absorption losses in any intermediate layers that might be needed. The EQE of the silicon single junction cell is limited also by front side reflection losses (measured against air in the single junction device). Of course the reflection between the perovskite and silicon cells will be slightly different, but as an approximation the original reflection values of the silicon cell are taken as an estimate. The two-terminal tandem device is limited by the lowest current density of the sub-cells, while the voltage is given by the sum of the voltages of the sub-cells. The results of the estimate are summarized in Table 12. The silicon bottom cell strongly limits the current density of the whole device. For an assumed fill factor of the tandem device of 85\%, an efficiency of 20.4\% can be reached. By adding the sphere grating, the current density of the whole device is raised by 1.3 mA/cm\(^2\), which increases the efficiency to 22.4\%. As expected, the efficiency gain of 2.0\% absolute is considerably larger than the efficiency gain for the single junction cell (0.8\%), which shows that diffractive gratings could be a promising structure for perovskite-silicon tandem devices. Note that there are other possible approaches to realize better current matching like using a thinner top cell or increasing the bandgap of the top cell. However, those approaches merely represent a redistribution of short-wavelength photons, while the proposed light trapping enhancement due to the sphere grating actually increases the overall number of utilized photons. Of course both approaches can be combined in the future. Additionally the transmittance of the top cell is of great importance. Assuming that all light for wavelengths larger than 600 nm that is not absorbed in the perovskite absorber is transmitted through the top cell - a highly
Comparison and evaluation of different light trapping structures

idealized assumption described by eq. (67) - results in overall efficiencies that are approximately 4% absolute higher. The resulting parameters for this case of improved transmission are also given in Table 12. Also the gain due to the spheres in this case is slightly higher because overall more photons are reaching the rear side of the bottom cell. [128]

6.3.2 III/V on Silicon

For a performance estimate of a III/V-Si tandem device, I refer to the work of Essig et al. [135]. They fabricated a triple junction device consisting of a GaInP/GaAs dual junction top cell that was wafer bonded onto a 280 µm thick silicon bottom cell. The current densities reached with this concept in the individual sub-cells are shown in Table 12. Again, the current density generated in the silicon bottom cell limits the whole device. Assuming a sphere grating rear side, the current of the silicon bottom cell can be increased by 1.1 mA/cm². The current density increase here is slightly lower due to the higher cell thickness and was estimated by simulations using OPTOS. Thus the silicon bottom cell would not limit the current anymore and the efficiency of the total device would be increased from 25.2 to 27.6% (2.4% absolute), demonstrating again the potential benefit of near infrared light trapping in Si-based tandem devices. [128]

Table 12: Estimated cell parameters of individual sub-cells in a perovskite-silicon tandem cell and a GaInP/GaAs-silicon triple cell. [128]

<table>
<thead>
<tr>
<th>Sub-cell Type</th>
<th>$J_{sc,\text{top}}$ [mA/cm²] (no spheres)</th>
<th>$J_{sc,\text{bottom}}$ [mA/cm²] (no spheres)</th>
<th>$J_{sc,\text{bottom}}$ [mA/cm²] (spheres)</th>
<th>$\eta$ [%] (no spheres)</th>
<th>$\eta$ [%] (spheres)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Perovskite-Silicon (real devices)</td>
<td>21.9</td>
<td>13.2</td>
<td>14.5</td>
<td>20.4¹</td>
<td>22.4¹</td>
</tr>
<tr>
<td>Perovskite-Silicon (improved transmission)</td>
<td>21.9</td>
<td>15.7</td>
<td>17.1</td>
<td>24.3</td>
<td>26.5</td>
</tr>
<tr>
<td>GaInP/GaAs-Silicon</td>
<td>11.0²; 12.0³</td>
<td>10.2</td>
<td>11.3</td>
<td>25.2⁴</td>
<td>27.6⁴</td>
</tr>
</tbody>
</table>

¹ $V_{OC}$ of total device is 1.81 V, assumed FF of 85 %.
² $J_{sc}$ of GaInP top cell
³ $J_{sc}$ of GaAs middle cell
⁴ $V_{OC}$ of total device is 2.88 V, FF is 87.1 %.
Summary

Silicon solar cells require light trapping structures, because silicon as indirect semiconductor only weakly absorbs light, especially in the near infrared (NIR) close to the bandgap of silicon. Such light trapping structures can be realized either on the front, where they have to fulfill also antireflective properties, or at the rear. To increase the overall efficiency of a complete device, in both cases not only the optical but also the electrical properties have to be optimized. The focus of this work was the simulation and experimental realization of novel light trapping structures, especially diffractive gratings, in high-efficiency crystalline silicon solar cells.

State-of-the-art structures like random pyramids at the front can be described in the regime of geometrical optics (e.g. by ray tracing). To describe gratings, which have been proposed for the use in crystalline silicon solar cells for decades, wave optical methods (e.g. rigorous coupled wave analysis, RCWA) have to be applied. If structures operating in different optical regimes are applied at front and rear surface, there has been no single simulation technique that can efficiently and correctly describe the complete system. Therefore, the simulation formalism **Optical Properties of Textured Optical Sheets (OPTOS)** was developed within this work (together with Nico Tucher within his dissertation). It allows for an efficient coupling of different simulation techniques for front and rear textures. Thus, most suitable methods can be applied for different surfaces in order to calculate light redistribution matrices, which are then coupled incoherently in a matrix-based formalism that is efficient with respect to computational effort. OPTOS allows for the calculation of all relevant optical properties like absorptance, reflectance, transmittance and also of a depth-dependent generation profile that can be used as input for subsequent electrical cell simulations. Also polarization-dependent effects are included in the matrices. The light redistribution matrices can be re-used and thus various combinations of front and rear textures and cell thicknesses can be calculated efficiently. OPTOS has been validated by comparison to existing simulations methods for systems that can be described within one optical regime and by comparison to measurements. The methodology of OPTOS has been published in three joint journal papers together with Nico Tucher [84–86] and a basic version of the code has been made available on the Fraunhofer ISE website¹ and on the platform PV Lighthouse².

Front side structures were investigated with respect to their antireflective and light trapping properties together with Alexander Bett within his master thesis [90]. All dielectric layers available at Fraunhofer ISE were used to optimize single, double and triple layer antireflection coatings – not only for solar cells but also for modules with an additional encapsulation material and glass on top. In simulations

¹ www.ise.fraunhofer.de/optos
and measurements, it was shown that with a double layer antireflection coating made of SiO$_2$ and TiO$_2$, averaged reflectivities down to 3.6% are possible. As materials with higher refractive indices than TiO$_2$ strongly absorb light at least in the short wavelength range, triple layer ARCs are only slightly superior to double layer ARCs and reach reflectivities down to 3.3%. With black silicon, significantly lower values down to 1.2% were demonstrated. Important for the combination with additional light trapping structures at the rear are the light redirecting properties of the front structure. For black silicon, detailed RCWA calculations revealed that significantly less light is scattered into large angles in forward direction compared to a Lambertian scatterer. Thus, the investigated black silicon surface itself is not sufficient to reach very good light trapping and a combination with an additional rear side structure can be beneficial, which was demonstrated in optical measurements. The results of the investigation of black silicon have been published together with Alexander Bett [91].

Structures for the rear, especially diffractive gratings, have been successfully integrated into high-efficiency crystalline silicon solar cells within this work. **Binary crossed gratings** with a period of 1 µm, fabricated via nanoimprint lithography and etching, have been applied to p-type silicon solar cells. A planar, 10 nm thin Al$_2$O$_3$ layer at the rear allows for very good electrical passivation and the grating is etched into amorphous silicon that has been sputter-deposited on top of the Al$_2$O$_3$ without deteriorating the electrical passivation quality. Local contacts through the grating and passivation layer have been realized with foil-based laser fired contacts. Thus, electrically planar and optically structured (EPOS) solar cells have been realized. $V_{OC}$ values of up to 683 mV, fill factors of 81% and efficiencies of up to 19% have been reached for 250 µm thick cells featuring a grating and a planar front. Compared to reference solar cells without grating, no voltage or fill factor loss was observed and the short circuit current density has been increased by 1.2 mA/cm$^2$ due to the grating. For thinner solar cells with thicknesses of 150 and 100 µm, this gain increased to 1.6 and 1.8 mA/cm$^2$, respectively. This $J_{SC}$-gain has been observed in IV- as well as in EQE-measurements. The EQE is in accordance to OPTOS simulations of the cells assuming a 10% parasitic loss at the rear surface of the cell, which might be attributed to parasitic absorption in the amorphous silicon or in the Al-foil. Reducing this parasitic absorption loss would allow for even higher enhancements of EQE and $J_{SC}$. For cells with an inverted pyramid texture at the front, the gain due to the grating has been found to be much less distinct – in accordance to theory and simulations. An EQE gain related to a current density gain of approx. 0.3 mA/cm$^2$ has been measured and leads to an overall efficiency of 21.1% for a 100 µm thin cell featuring inverted pyramids at the front and a binary grating at the rear. The results of binary gratings integrated into p-type silicon solar cells have been published [123].

Also hexagonal **sphere gratings** (sphere diameter 0.966 µm) have been successfully integrated into high-efficiency crystalline silicon solar cells. By using n-type solar cells with a tunnel oxide passivated contact (TOPCon) at the rear and an additional sphere grating structure on top of TOPCon, again EPOS solar cells have been realized. The sphere grating fabrication consists of two main steps:
first, spin coating of monodisperse SiO\textsubscript{2} spheres leading to a dense, hexagonally ordered monolayer and second, filling of the voids in between the spheres with doped poly-crystalline silicon using atmospheric pressure chemical vapor deposition. On top, an ITO and Ag layer complete the full area passivated rear side contact. Due to a hydrogen annealing step after the poly-crystalline silicon deposition, the passivation quality of the TOPCon layer system was preserved as shown in life time measurements. For cells with a thickness of 200 µm and a planar front surface, this approach allowed for a $V_{OC}$ of 710 mV, a fill factor of 81.9%, a $J_{SC}$ of 38.1 mA/cm\textsuperscript{2} and thus an efficiency of 22.1%. Similar to the cells with binary gratings, the optical effect of the sphere gratings can be observed in IV-measurements but is especially visible in EQE-measurements. It corresponds to a current density gain of 1.4 mA/cm\textsuperscript{2}. Comparing the EQE measurements to OPTOS simulations, revealed that also for the sphere grating, parasitic absorption in the rear structure reduces the beneficial effect of the grating, which has already been indicated by optical measurements. Adapting the doping profile of the polycrystalline matrix to a variable and overall lower doping level allowed for a reduction of the parasitic absorption from 20 to 10%. However, for solar cells with textured front surface, the parasitic absorption still compensates the improved light trapping and no overall EQE gain has been observed. Similar to binary gratings, a reduction of parasitic absorption in the sphere grating would allow for even higher gains in solar cells with planar front and also for gains in solar cells with random pyramids at the front. Major results of the integration of sphere gratings into high-efficiency crystalline silicon solar cells have been published in a journal publication originated from a contribution to Silicon PV [128].

Both grating types can be benchmarked to a simple rear structure: an externally applied diffuse scatterer like white paint or TiO\textsubscript{2} nanoparticles. These simple rear structures have been investigated together with Florian Pfeffer within his bachelor thesis and results have been published [104]. For solar cells with a thickness of 250 µm and a planar front surface, white paint allows for a $J_{SC}$ gain of up to 0.8 mA/cm\textsuperscript{2} compared to an externally applied high-quality silver mirror. Thus, the developed diffractive gratings lead to significantly better light trapping than a diffuse reflector applied externally to the rear side of silicon solar cells.

To overcome the limits of solar cells featuring one single pn-junction, tandem solar cells are a promising approach. Silicon based tandem devices are in the focus of research, as already developed standard silicon technology and industrial solutions can still be used. The light trapping structures for the rear of crystalline silicon solar cells developed and investigated in this work can be of special importance for silicon based tandem devices for two reasons: first, many concepts require a planar front surface of the silicon bottom solar cell and second, devices reported so far often suffer from low absorption in the silicon bottom solar cell. Increasing the absorption in the NIR due to a rear grating would increase the $J_{SC}$ of the complete tandem device. Approximations based on the sphere grating results achieved in this work and literature values for III-V and perovskite cells show that applying a
grating to a III-V on silicon or perovskite on silicon tandem device can increase the efficiency by more than 2% absolute, compared to 0.8% reached within this work for a single junction silicon solar cell.

gemeinsam mit Nico Tucher veröffentlicht [84–86] und eine Basisversion des Quellcodes wurde auf der Homepage des Fraunhofer ISE\(^1\) sowie bei PV Lighthouse\(^2\) zur Verfügung gestellt.


Strukturen für die Zellrückseite, insbesondere Beugungsgitter, habe ich im Rahmen dieser Arbeit erfolgreich in hocheffiziente kristalline Siliziumsolarzellen integriert. Binäre Gitter mit einer Periode von 1 \(\mu\)m, hergestellt mittels Nanoimprintlithographie und Ätzprozessen, wurden auf der Rückseite von p-typ Solarzellen realisiert. Eine plane, 10 nm dünne Al\(_2\)O\(_3\) Schicht ermöglicht eine sehr gute elektrische Passivierung und das Gitter wird in eine amorphe Siliziumschicht geätzt, die mittels Sputtern auf das Al\(_2\)O\(_3\) abgeschieden wurde, ohne dabei die passivierenden Eigenschaften zu verschlechtern. Mittels folienbasierten, lasergefeuerten Kontakten wurden durch Gitter und Passivierschicht hindurch lokale elektrische Kontakte hergestellt. Somit weisen die Solarzellen elektrisch plane und optisch strukturierte Grenzflächen auf. Offenklemmspannungen von bis zu 683 mV, Füllfaktoren bis 81% und Effizienzen bis zu 19% wurden für 250 \(\mu\)m dicke Solarzellen mit binärem Beugungsgitter und planer Vorderseite erreicht. Im Vergleich zu Referenzzellen ohne Gitter konnte weder eine Reduktion des Füllfaktors noch der Offenklemmspannung festgestellt werden. Der Kurzschlussstrom \(J_{sc}\) jedoch konnte durch das Gitter um 1.2 mA/cm\(^2\) gesteigert werden. Für dünnere

\(^1\) www.ise.fraunhofer.de/optos

Kurzschlussstroms erreicht werden. Die wichtigsten Ergebnisse zur Integration von Kugelgittern in hocheffiziente, kristalline Siliziumsolarzellen wurden veröffentlicht [128].

Beide Gitterarten können als Bezugspunkt mit einer einfachen Rückseitenstruktur verglichen werden: einem extern auf der Zellrückseite aufgebrachten diffusen Streuer wie z.B. weißer Farbe oder TiO$_2$-Nanopartikeln. Diese Art von Rückseitenstruktur wurde gemeinsam mit Florian Pfeffer im Rahmen seiner Bachelorarbeit untersucht und die Ergebnisse wurden veröffentlicht [104]. Für Solarzellen mit einer Dicke von 250 µm und planer Vorderseite wurde durch eine Rückseite mit weißer Farbe im Vergleich zu einem hochwertigen externen Silberspiegel ein Kurzschlusstromgewinn von 0.8 mA/cm$^2$ erreicht. Dies zeigt, dass die entwickelten, integrierten Beugungsgitter einen signifikant besseren Lichteinfang ermöglichen als diffuse Streuer, die extern an der Rückseite von Solarzellen angebracht werden.

Literature

11. M. A. Green, *Silicon solar cells. advanced principles and practice* (Centre for Photovoltaic Devises and Systems UNSW, 1995).
26. “PV Lighthouse OPAL 2 Calculator,”


Appendix

A) Unit cell effects in the RCWA simulation of black Si

The discrete angular distribution within the Si bulk, composed of propagating modes that are induced by the artificially introduced periodicity, can lead to significant unit cell effects in the transmittance spectra. For a given unit cell size, depending on the wavelength, more or less modes can propagate. Some of the modes correspond to polar angels below the critical angle such that the light can leave the silicon at the rear side, while other modes are trapped by total internal reflection. Significant steps can be seen in the transmittance spectra at the wavelength where a mode overcomes the limit from transmission to total internal reflection. With increasing unit cell size these effects decrease because the number of propagating modes increases and thus a single mode is less important. As it is crucial for the used method to understand possible unit cell effects, Figure 86 shows differences between the simulated and measured transmittance for further different unit cell sizes. 15 random structures were considered for every period with the exception of the largest unit cell, where only 10 structures were taken into account due to the high computational effort. For periods of 1.35 µm and 1.40 µm the simulated spectra match the measured data within the statistical error. For the three subsequent unit cell sizes with periods of 1.46 µm, 1.49 µm and 1.54 µm, the simulated transmittance is significantly higher than the measured values at the beginning of the spectral range considered. With increasing wavelength, the differences vanish one by one. For the periods of 1.59 µm and 1.70 µm the simulated transmittance is too high compared to the measurement data, but with increasing unit cell size the difference decreases and for a period of 2.01 µm the simulated spectrum matches the measured curve well again. [91]

![Figure 86: Difference between simulated and measured transmittance for different periods. [91]](image-url)
To explain the curve progressions in Figure 86, one has to consider the polar angles of the propagating modes. Each propagating mode has a certain azimuth and polar angle. By integration over the azimuth angle, the intensity occurring under a certain polar angle can be calculated. The discrete set of modes results in a discrete set of polar angles. Table 13 contains the number of different polar angles for which propagating modes exist for all periods considered in Figure 86 and for three different wavelengths. The critical polar angle separating the loss cone from the solid angle of total internal reflection at the rear side is 16.27° at a wavelength of 1.00 µm, 16.33° at 1.04 µm and 16.38° at 1.08 µm. Within the loss cone (for polar angles below the critical angle), light can leave the silicon bulk at the rear side; for higher angles light is totally internally reflected. In Table 13, also the number of polar angles for which propagating modes exist that are below the critical angle is listed. For the two smallest unit cells of periods 1.35 µm and 1.40 µm for two polar angles within the loss cone propagating modes exists, and modes associated with the third polar angle are already subjected to total internal reflection. For a period of 1.46 µm and a wavelength of 1.00 µm, three polar angles occur that are smaller than the critical angle, thus leading to out-coupling of the associated propagating modes. Hence, the transmittance is higher than for the smaller periods. At a wavelength of 1.04 µm only two polar angles occur that are smaller than the critical angle, thus the transmittance decreases. For a larger period of 1.49 µm, the transition between 3 and 2 occurring polar angles below the critical angles, takes place at a higher wavelength. Therefore, in Figure 86 one can see a decrease in transmittance between 1.04 µm and 1.08 µm. The angular distributions for a period of 1.49 µm are shown in Figure 87. With further increasing the period, the difference between the simulated and measured transmittance decreases, because the larger the unit cell, the more propagating modes exist altogether and the smaller the influence of one single mode. For the largest unit cell considered with a period of 2.01 µm the measurement data are matched well by the simulation. One can conclude that for simulation, unit cells of a period of at least 2 µm have to be used to get rid of unit cell effects. [91]
Table 13: Number of polar angles associated with propagating modes and number of polar angles associated with propagating modes smaller than the angle of total internal reflection for different wavelengths.

<table>
<thead>
<tr>
<th>Period (µm)</th>
<th>Number of polar angles associated with propagating modes</th>
<th>Wavelength 1.00 µm &lt; 16.27°</th>
<th>Wavelength 1.04 µm &lt; 16.33°</th>
<th>Wavelength 1.08 µm &lt; 16.38°</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.35</td>
<td>13 2</td>
<td>13 2</td>
<td>12 2</td>
<td></td>
</tr>
<tr>
<td>1.40</td>
<td>14 2</td>
<td>13 2</td>
<td>13 2</td>
<td></td>
</tr>
<tr>
<td>1.46</td>
<td>15 3</td>
<td>15 3</td>
<td>13 2</td>
<td></td>
</tr>
<tr>
<td>1.49</td>
<td>15 3</td>
<td>15 3</td>
<td>13 2</td>
<td></td>
</tr>
<tr>
<td>1.54</td>
<td>16 3</td>
<td>15 3</td>
<td>14 3</td>
<td></td>
</tr>
<tr>
<td>1.59</td>
<td>17 3</td>
<td>16 3</td>
<td>15 3</td>
<td></td>
</tr>
<tr>
<td>1.67</td>
<td>18 3</td>
<td>17 3</td>
<td>16 3</td>
<td></td>
</tr>
<tr>
<td>2.01</td>
<td>24 4</td>
<td>23 3</td>
<td>22 3</td>
<td></td>
</tr>
</tbody>
</table>

Figure 87: Angular distributions for a period of 1.49 µm at wavelengths of 1.04 µm and 1.08 µm. At 1.04 µm three polar angles associated with propagating modes are smaller than the critical angle marked by the vertical line. At a wavelength of 1.08 µm only two polar angles corresponding to propagating modes are within the loss cone. [91]
### B) Acronyms

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>a-Si</td>
<td>Amorphous silicon</td>
</tr>
<tr>
<td>Ag</td>
<td>Silver</td>
</tr>
<tr>
<td>ALD</td>
<td>Atomic layer deposition</td>
</tr>
<tr>
<td>Al</td>
<td>Aluminum</td>
</tr>
<tr>
<td>Al₂O₃</td>
<td>Aluminum oxide</td>
</tr>
<tr>
<td>ARC</td>
<td>Anti-reflective coating</td>
</tr>
<tr>
<td>APCVD</td>
<td>Atmospheric pressure chemical vapor deposition</td>
</tr>
<tr>
<td>BSF</td>
<td>Back surface field</td>
</tr>
<tr>
<td>c-Si</td>
<td>Crystalline silicon</td>
</tr>
<tr>
<td>DARC</td>
<td>Double layer ARC</td>
</tr>
<tr>
<td>DBL</td>
<td>Dielectric buffer layer</td>
</tr>
<tr>
<td>EPOS</td>
<td>Electrically planar and optically structured</td>
</tr>
<tr>
<td>EVA</td>
<td>Ethylvinylacetate</td>
</tr>
<tr>
<td>FCA</td>
<td>Free carrier absorption</td>
</tr>
<tr>
<td>FZ</td>
<td>Float zone</td>
</tr>
<tr>
<td>HF</td>
<td>Hydroflouric acid</td>
</tr>
<tr>
<td>ISE</td>
<td>Institute for Solar Energy Systems</td>
</tr>
<tr>
<td>IP</td>
<td>Inverted pyramids</td>
</tr>
<tr>
<td>ITO</td>
<td>Indium tin oxide</td>
</tr>
<tr>
<td>KOH</td>
<td>Potassium hydroxide</td>
</tr>
<tr>
<td>LFC</td>
<td>Laser fired contacts</td>
</tr>
<tr>
<td>MgF₂</td>
<td>Magnesium fluoride</td>
</tr>
<tr>
<td>MPP</td>
<td>Maximum power point</td>
</tr>
<tr>
<td>NaOH</td>
<td>Natrium hydroxide</td>
</tr>
<tr>
<td>NIL</td>
<td>Nanoimprint lithography</td>
</tr>
<tr>
<td>NIR</td>
<td>Near infrared spectral region (typically 800-1200 nm)</td>
</tr>
<tr>
<td>n-Si</td>
<td>n-doped silicon</td>
</tr>
<tr>
<td>OPTOS</td>
<td>Optical properties of textured optical sheets</td>
</tr>
</tbody>
</table>
### Appendix

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PDMS</td>
<td>Polydimethylsiloxane</td>
</tr>
<tr>
<td>PECVD</td>
<td>Plasma enhanced chemical vapor deposition</td>
</tr>
<tr>
<td>PERC</td>
<td>Passivated emitter rear contact</td>
</tr>
<tr>
<td>PERT</td>
<td>Passivated emitter rear totally diffused</td>
</tr>
<tr>
<td>pg</td>
<td>Planar front and grating rear</td>
</tr>
<tr>
<td>PL</td>
<td>Photolithography</td>
</tr>
<tr>
<td>pp</td>
<td>Planar front and planar rear</td>
</tr>
<tr>
<td>p-Si</td>
<td>p-doped silicon</td>
</tr>
<tr>
<td>RCWA</td>
<td>Rigorous coupled wave analysis</td>
</tr>
<tr>
<td>RP</td>
<td>Random pyramids</td>
</tr>
<tr>
<td>rpm</td>
<td>Rounds per minute</td>
</tr>
<tr>
<td>SARC</td>
<td>Single layer ARC</td>
</tr>
<tr>
<td>sccm</td>
<td>Standard cubic centimeters per minute</td>
</tr>
<tr>
<td>SEM</td>
<td>Scanning electron microscope</td>
</tr>
<tr>
<td>Si</td>
<td>Silicon</td>
</tr>
<tr>
<td>SiNₓ</td>
<td>Silicon nitride</td>
</tr>
<tr>
<td>SiO₂</td>
<td>Silicon dioxide</td>
</tr>
<tr>
<td>SRH</td>
<td>Shockley-Read-Hall recombination</td>
</tr>
<tr>
<td>STC</td>
<td>Standard testing conditions</td>
</tr>
<tr>
<td>tg</td>
<td>textured front and grating rear</td>
</tr>
<tr>
<td>tp</td>
<td>textured front and planar rear</td>
</tr>
<tr>
<td>tt</td>
<td>textured front and textured rear</td>
</tr>
<tr>
<td>TE</td>
<td>Transversal electric</td>
</tr>
<tr>
<td>TiO₂</td>
<td>Titanium dioxide</td>
</tr>
<tr>
<td>TM</td>
<td>Transversal magnetic</td>
</tr>
<tr>
<td>TMM</td>
<td>Transfer matrix method</td>
</tr>
<tr>
<td>TOPCon</td>
<td>Tunnel oxide passivated contact</td>
</tr>
<tr>
<td>UV</td>
<td>Ultra-violet</td>
</tr>
<tr>
<td>2D</td>
<td>two-dimensional</td>
</tr>
<tr>
<td>3D</td>
<td>three-dimensional</td>
</tr>
</tbody>
</table>
## C) Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Typical Unit</th>
<th>Quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>1/m</td>
<td>Absorptance</td>
</tr>
<tr>
<td>(\alpha)</td>
<td>1/m</td>
<td>Absorption coefficient</td>
</tr>
<tr>
<td>(\alpha_{FCA})</td>
<td>1/m</td>
<td>Free carrier absorption coefficient</td>
</tr>
<tr>
<td>(B_{int})</td>
<td>W/m²/sr</td>
<td>Internal intensity</td>
</tr>
<tr>
<td>(c_{azimuth})</td>
<td></td>
<td>Parameter for the azimuth angle discretization</td>
</tr>
<tr>
<td>(d)</td>
<td>m</td>
<td>substrate thickness</td>
</tr>
<tr>
<td>(D)</td>
<td></td>
<td>Propagation matrix</td>
</tr>
<tr>
<td>(D_{it})</td>
<td>1/m²</td>
<td>Interface trap density</td>
</tr>
<tr>
<td>(\delta)</td>
<td>m</td>
<td>penetration depth</td>
</tr>
<tr>
<td>(\Delta n)</td>
<td>1/cm³</td>
<td>Excess carrier density of electrons</td>
</tr>
<tr>
<td>(\Delta p)</td>
<td>1/cm³</td>
<td>Excess carrier density of holes</td>
</tr>
<tr>
<td>(E_G)</td>
<td>eV</td>
<td>Bandgap energy</td>
</tr>
<tr>
<td>(EQE)</td>
<td></td>
<td>External quantum efficiency</td>
</tr>
<tr>
<td>(\eta)</td>
<td></td>
<td>Solar cell efficiency</td>
</tr>
<tr>
<td>FF</td>
<td></td>
<td>Fill factor</td>
</tr>
<tr>
<td>(\theta)</td>
<td>rad or degree</td>
<td>Polar angle</td>
</tr>
<tr>
<td>(\theta_c)</td>
<td>rad</td>
<td>Critical angle for total internal reflection</td>
</tr>
<tr>
<td>(I)</td>
<td></td>
<td>Identity matrix</td>
</tr>
<tr>
<td>(I_{inc})</td>
<td>W/m²</td>
<td>Incident irradiance</td>
</tr>
<tr>
<td>(I_{int})</td>
<td>W/m²</td>
<td>Internal irradiance</td>
</tr>
<tr>
<td>(iV_{OC})</td>
<td>mV or V</td>
<td>Implied open circuit voltage</td>
</tr>
<tr>
<td>IQE</td>
<td></td>
<td>Internal quantum efficiency</td>
</tr>
<tr>
<td>(J_{SC})</td>
<td>mA/cm²</td>
<td>Short circuit current density</td>
</tr>
<tr>
<td>(J_0)</td>
<td>mA/cm²</td>
<td>Dark saturation current density</td>
</tr>
<tr>
<td>(J_L)</td>
<td>mA/cm²</td>
<td>Current density induced by light absorption</td>
</tr>
<tr>
<td>(J_{ph})</td>
<td>mA/cm²</td>
<td>Photo circuit current density</td>
</tr>
<tr>
<td>(k)</td>
<td>1/m</td>
<td>Refractive index (imaginary part)</td>
</tr>
<tr>
<td>(k)</td>
<td></td>
<td>Wave vector</td>
</tr>
</tbody>
</table>
Appendix

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Unit</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_{pq}$</td>
<td>1/m</td>
<td>Reciprocal lattice vector of order pq</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>$\mu$m or nm</td>
<td>Wavelength</td>
</tr>
<tr>
<td>$A$</td>
<td>$\mu$m</td>
<td>Grating constant</td>
</tr>
<tr>
<td>$m$</td>
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<td>Number of diffractive order</td>
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<td>$m_{max}$</td>
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<td>Maximum number of propagable orders</td>
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<tr>
<td>$n$</td>
<td></td>
<td>Refractive index (real part)</td>
</tr>
<tr>
<td>$n_i$</td>
<td>1/cm$^3$</td>
<td>Intrinsic charge carrier concentration</td>
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<tr>
<td>$N$</td>
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<td>Refractive index (complex)</td>
</tr>
<tr>
<td>$N_{AM15g}$</td>
<td>1/m$^3$</td>
<td>Spectral photon flux density of the AM15g spectrum</td>
</tr>
<tr>
<td>$N_{azimuth}$</td>
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<td>Number of azimuth intervals in each symmetry element for one polar angle</td>
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<tr>
<td>$\phi$</td>
<td>rad</td>
<td>Azimuth angle</td>
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<tr>
<td>$P$</td>
<td>W/m$^2$</td>
<td>Power density</td>
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<tr>
<td>$P_{MPP}$</td>
<td>W/m$^2$</td>
<td>Power density at maximum power point</td>
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<tr>
<td>$q$</td>
<td>C</td>
<td>Elementary charge</td>
</tr>
<tr>
<td>$R$</td>
<td></td>
<td>Reflectance</td>
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<tr>
<td>$R$</td>
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<td>Reflection matrix</td>
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<tr>
<td>$S$</td>
<td>cm/s</td>
<td>Recombination velocity</td>
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<tr>
<td>$\tau$</td>
<td>s</td>
<td>Charge carrier recombination lifetime</td>
</tr>
<tr>
<td>$\tau_{eff}$</td>
<td>s</td>
<td>Effective charge carrier recombination lifetime</td>
</tr>
<tr>
<td>$T$</td>
<td></td>
<td>Transmittance</td>
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<tr>
<td>$T$</td>
<td></td>
<td>Transmission matrix</td>
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<tr>
<td>$U$</td>
<td>1/s</td>
<td>Recombination rate</td>
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<tr>
<td>$v$</td>
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<td>Power distribution vector</td>
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<tr>
<td>$V$</td>
<td>mV or V</td>
<td>Voltage</td>
</tr>
<tr>
<td>$V_{OC}$</td>
<td>mV or V</td>
<td>Open circuit voltage</td>
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<td>$w$</td>
<td>$\mu$m</td>
<td>Solar cell thickness</td>
</tr>
<tr>
<td>$\Omega$</td>
<td>sr</td>
<td>Solid angle</td>
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</table>
Appendix

D) Author’s publications

Reviewed journal papers


Conference papers


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