OPTICS IN THIN-FILM SILICON SOLAR CELLS WITH PERIODIC SURFACE TEXTURE

by

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Chapter 1

Introduction

1.1 Motivation

Photovoltaic solar cells can play an important role in meeting the ever increasing demand for energy. With the global energy scarcity that our society faces, the growing interest in renewable energy sources is quite evident worldwide. In the year 2010 itself with an installation of 16.6 gigawatts, the photovoltaic market doubled compared to the previous year when capacity of 7.2 gigawatts was installed [1]. Photovoltaic technology harnesses, the freely available and emission free, sunlight and converts it to electricity for our usage.

Thin-film solar cells are promising candidates for future generations of photovoltaic devices [2]. Whilst current industry standard solar cells use wafer-based silicon (more than 80 % of the market) [3], an obvious way forward is to reduce the material cost by using thin-film technology. Thin-film solar cells are usually deposited on low cost substrates such as glass or plastic [4]. With a much lower fabrication cost for these thin-film solar cells, the industry for thin-film devices can be promising if their conversion efficiencies or in turn their price per watt are competitive compared to the price per watt of wafer based silicon solar cells. The absorber material in thin-film solar cells are mostly based on: amorphous silicon (a-Si), microcrystalline silicon (µc-Si), copper indium deselenide (CIS/CIGS) and cadmium telluride (CdTe). In this work the main focus is on the analysis of thin-film solar cells based on hydrogenated microcrystalline silicon. Thin-film microcrystalline silicon solar cells have a typical thickness of 0.8–1.5 μm, which is significantly less than the thickness of conventional wafer based silicon solar cells (180–250 μm) [5].

Reducing the cost and increasing the conversion efficiency is a major objective of research and development for thin-film silicon solar cells. An approach that simultaneously achieves these two objectives is to use light-trapping or photon management. Light trapping facilitates the absorption of sunlight by a thin-film solar cell that is much
1. Introduction

Thinner than the absorption length of the material. Over the last decade, several concepts have been proposed to enhance the absorption of light in thin-film silicon solar cells. Most of the concepts are based on random nanotexturing of the contact layers of the solar cells. Conversion efficiencies higher than 10% have been demonstrated for amorphous and thin-film microcrystalline silicon solar cells by introducing randomly textured interfaces in the solar cell [6, 7]. For micromorph (amorphous and microcrystalline silicon) tandem solar cells stable efficiencies of up to 11.9% have been demonstrated using textured interfaces [8]. The introduction of textured interfaces reduces reflection losses and enhances light scattering and diffraction within the device. Due to multiple reflections within the silicon layer the optical path length of the incident light is greatly enhanced. This leads to a significantly enhanced short circuit current and quantum efficiency in the red and infrared part of the optical spectrum.

1.2 Outline of the Thesis

In order to understand the optical propagation within such thin-film devices, it is imperative to use numerical methods and solve the Maxwell’s equations rigorously. The finite difference time domain method, finite element method, or rigorous coupled wave analysis are commonly used to simulate the near-field and far-field wave propagation in such devices [9–13]. By considering the near field optics, the nanotexturing process for efficient solar cells can be understood and optimized. Within the scope of this thesis, the optical enhancement and losses of microcrystalline thin-film silicon solar cells with periodic surface textures were investigated. Beginning with a simplified grating structure, the investigation in this work sequentially moved onto investigating the influence of 3-dimensional pyramid textures on the optical wave propagation in the thin-film devices. The different design parameters and methods are discussed in the different chapters of this thesis. This thesis has been organized in such a way that each of the chapters can be read as stand alone chapters as well. The structure of the thesis is briefly described in the following:

In chapter 2, the key parameters that entail the study of thin-film silicon solar cells are described. The optical properties of the different materials in the stratified thin-film solar cell stack are discussed. Understanding these properties and how these optical properties interact together in a solar cell is essential for optimization towards efficient solar cells. Theoretical limits on the absorption enhancement and efficiency of solar cells are derived, which serve as a benchmark for comparing the results in the later chapters. The commonly used light confinement techniques in research and production are also described.

In chapter 3, the algorithms for the numerical methods used in this study are described. A brief recap on the fundamentals of electromagnetics theory was presented
which preceded the description of the Maxwell’s solvers methods, namely finite difference time domain and rigorous coupled wave analysis.

In chapters 4-7, the simulation results from this study are presented and discussed. Each of the chapters begin with a description of the simulation model used for computation in that chapter. The results from every chapter were discussed independently of the others. The finite difference time domain method was utilized for the computation in chapters 4, 5 and 7. And for chapter 6, the computation method was rigorous coupled wave analysis. In these chapters, the influence of the period and height of the surface texture on the quantum efficiency and short circuit current of the solar cell was investigated. The trends in the optical behavior were understood by using theories of optics and subwavelength optics.

In chapter 8, the important results from the preceding chapters were summarized. An outlook to future directions of research is also discussed.
Chapter 2

Fundamental Concepts

Understanding of the optical properties of the materials used in solar cells are pivotal in order to design and optimize efficient devices. In this chapter, the basics involving device physics of thin-film solar cells and the optical properties of doped zinc-oxide, amorphous and microcrystalline silicon are briefly discussed. Starting with the characteristics output parameter of solar cells, we conclude this chapter with a discussion on textured substrates and its application as templates for light trapping structures in thin-film silicon solar cells.

2.1 Characteristic Parameters of Solar Cells

Solar cells are optoelectronic devices which generate both the current and voltage to supply with electric power. A precondition to this generation of energy is that the solar cell needs to be illuminated by light. Assuming ideal $I-V$ characteristics, a p-n junction solar cell (which is in principle not different from a diode) can be represented as an equivalent circuit with a constant current source of photocurrent which is in parallel to the diode junction. The current voltage characteristics equation for an ideal solar cell is given by

$$I = I_S \left[ \exp \left( \frac{qV}{kT} \right) - 1 \right] - I_L$$

(2.1)

where $I_S$ and $I_L$ are the saturation and light generated current of the diode, respectively. $q$ is the elementary charge, $k$ is Boltzmann constant, $T$ is the temperature of the solar cell in consideration and $V$ is the applied voltage. Illumination of light shifts the $I-V$ curve of the dark solar cell with the light generated current into the fourth quadrant [14]. The greater the intensity of the incident light, the greater the amount of light generated current.

Now, there are three important solar cell parameters which can be determined from the $I-V$ curve. They are: short circuit current, $I_{SC}$, open-circuit voltage, $V_{OC}$ and fill
2. FUNDAMENTAL CONCEPTS

Figure 2.1: (a) I-V characteristic of a solar cell in dark and under illumination conditions. (b) Output power curve for the corresponding solar cell under illumination. The characteristic parameters of a solar cell are also highlighted in the figure.

factor, $FF$. The I-V curve of a solar cell, along with these parameters, is shown in Fig. 2.1(a). And the output power from the corresponding solar cell under illumination as a function of the bias voltage is also shown in Fig. 2.1(b). Short circuit current is generated due to the generation and collection of photon-generated carriers (when no voltage is produced between the anode and cathode). And ideally, this current $I_{SC}$ is equal to the illumination current $I_L$, i.e. it is the largest current that can be drawn from a solar cell. $V_{OC}$ is the maximum possible voltage available from the solar cell. The voltage of the solar cell reaches the open circuit voltage for current flow of $I = 0$. From Eq. 2.1 it can be derived that for a given illumination current $I_L$, the open circuit voltage increases logarithmically with decreasing saturation current $I_S$.

Even though $I_{SC}$ and $V_{OC}$ are the maximum possible current and voltage obtainable from the solar cell, the power obtained at these two points are zero. In Fig. 2.1 the operating point that generates the maximum power ($P_{mp} = V_{mp}I_{mp}$) that can be obtained from the solar cell is also highlighted. Therefore, the maximum thermodynamic efficiency $\eta$ of the photovoltaic energy conversion process for a solar cell is:

$$\eta = \frac{V_{mp}I_{mp}}{P_{IN}} \quad (2.2)$$
where $P_{IN}$ is the total incident power. We can also observe from Fig. 2.1 that for an ideally shaped $I-V$ curve, it would look rectangular. Which means the solar cell would deliver a constant current density $I_{SC}$ until the open voltage $V_{OC}$. The term called the fill factor ($FF$) has been introduced to measure how close a given characteristic curve of a solar cell is to the ideal rectangular $I-V$ shape. Together with $I_{SC}$ and $V_{OC}$, the $FF$ is defined by the following ratio

$$FF = \frac{V_{mp}I_{mp}}{V_{OC}I_{SC}}$$ (2.3)

By definition, $FF \leq 1$. By inserting the relationship from Eq. 2.3 into Eq. 2.2, we obtain

$$\eta = \frac{V_{OC}I_{SC}FF}{P_{IN}}$$ (2.4)

Along with the three output characteristic parameters of the solar cell, the previous equation defining the efficiency of a solar cell is the most commonly utilized quantity to measure the performance of solar cells.

### 2.1.1 Shockley-Queisser Efficiency Limit

In the last five decades, several authors have studied the efficiency limits of solar cells using different hypothesis on the optical and electrical losses from the solar cell, and have published the efficiency limits for single junction or multi-junction solar cells [15–22]. But due to its simplicity in formalizing the problem, the paper on detailed balance efficiency limits published in 1961 by Shockley and Queisser still provides the benchmark for evaluating the performance of a single junction solar cell [15]. Shockley and Queisser calculated the maximum efficiency of solar cells by only taking the fundamental radiative recombination losses into account.

In their work, they assumed the sun and the solar cell in consideration to be two thermodynamic bodies with temperatures of 6000 K and 300 K, respectively. Thus the spectral density of the incident power used in Shockley and Queisser’s work followed the blackbody radiation which is described by the Planck’s law. But due to scattering, absorption and reflection in the atmosphere, sunlight that reaches the Earth’s surface is reduced in power. Therefore in this section we consider the current standard spectral densities for sunlight, namely AM 0 and AM 1.5\(^1\). The solar radiation just outside the earth’s atmosphere is called AM 0, where the losses are primarily caused by the ultraviolet absorption in ozone and infrared absorption in water vapor. The incident power for AM 0 illumination is approximately 1.353 kW/m\(^2\). For solar cell performance

\(^1\)When the sun is at angle $\theta$ to overhead, the air mass (AM) is given by: $AM = \frac{1}{\cos \theta}$. E.g. when the sun is $48.2^\circ$ off overhead, the radiation is AM 1.5.
comparisons that are tested at different locations, a terrestrial standard has been
defined to be AM 1.5 radiation, as the total incident power for AM 1.5 illumination is 1
kW/m². The spectral distributions of sunlight for AM 0 and AM 1.5 radiation, which
are considered in this section, are shown in Fig. 2.3(a).

The calculation of the efficiency limit is based on the following hypothesis (as stated
in the original paper):

“Each photon with energy greater than $h\nu_g$ produces one electronic
charge $q$ at a voltage of $V_g = h\nu_g/q$.”

Where $q$ is the elementary charge and the bandgap, $E_g$ of the material is related to
Planck constant, $h$ and frequency of the photon, $\nu$ as $E_g = h\nu_g$. Now, in order to derive
the current-voltage relationship of the solar cell after considering recombination losses,
five processes have to be considered.

1. Generation rate of electron-hole pairs by the solar illumination, $G_S$.
2. Radiative recombination loss from the solar cell, $R_R$.
3. Non-radiative generation processes, $G_{NR}$.
4. Non-radiative recombination processes, $R_{NR}$.
5. Extraction of electron-hole pairs as current flow $I$ at the rate of $I/q$.

We start with the thermal equilibrium condition. Under thermal equilibrium condi-
tions, when the solar cell can be assumed to be surrounded by a blackbody of its own
temperature, photons with energy higher than $E_g$ will be incident on the solar cell at
a rate which can be calculated by the blackbody radiation formula. For a solar cell
body being illuminated at area $A$, this generation rate due to absorption of photons in
thermal equilibrium can be expressed as

$$G_0(\nu, T) = A\frac{2\pi}{c^2} \int_{\nu_g}^{\infty} \frac{\nu^2}{\exp(\frac{h\nu}{kT}) - 1} d\nu$$ (2.5)

where $c$ is the speed of light, $k$ is the Boltzmann constant and $T$ is the temperature
of the solar cell in consideration. The subscript 0 denotes thermal equilibrium. By
considering a unit area of illumination and rewriting the expression in terms of the
energy bandgap, we obtain

$$G_0(E, T) = \frac{2\pi}{h^3c^2} \int_{E_g}^{\infty} \frac{E^2}{\exp(\frac{E}{kT}) - 1} dE$$ (2.6)
2.1. Characteristic Parameters of Solar Cells

Figure 2.2: Band diagram of a p-n junction in (a) thermal equilibrium and (b) under illumination conditions. Under thermal equilibrium the built-in potential of $V_{bi}$ corresponds to energy of $qV_{bi}$, where $q$ is the elementary charge. Under illumination, the Fermi level is split and quasi Fermi levels separated by a potential of energy $qV$ are created.

Following the generation rate in thermal equilibrium, we need to find the fundamental losses in the solar cell due to radiative recombination. We know from classical device physics that in thermal equilibrium, the generation and recombination rate due to photon absorption and emission are equal. Thus the radiative recombination under thermal equilibrium, $R_{R0}$ can be expressed in terms of Eq. 2.6 as well. Therefore,

$$R_{R0}(E, T) = G_0(E, T)$$ \hspace{1cm} (2.7)

The band diagrams of a p-n junction for both under thermal equilibrium and under illumination is shown in Fig. 2.2. In thermal equilibrium condition there is only a single Fermi level for the entire p-n junction where the energy bands bend with a built in potential of voltage $V_{bi}$. Under illumination from external source, the Fermi level is split and quasi Fermi levels are created for holes and electrons which are separated by a voltage $V$. This voltage $V$ is also the voltage between the external terminals to the solar cell. Now, the recombination rate is proportional to the product of the electron ($n$) and hole ($p$) concentration, i.e. $R_{R0} \propto np$. In thermal equilibrium conditions this means that $R_{R0} \propto n_i^2$, where $n_i$ is the intrinsic carrier concentration. Thus the recombination rate due to illumination, when the thermal equilibrium condition is disturbed, can be expressed as
2. **Fundamental Concepts**

\[
R_R(E, T) = \frac{R_{R0} np}{n_i^2} \tag{2.8}
\]

\[
R_R(E, T, V) = R_{R0}e^{\frac{qV}{kT}} \tag{2.9}
\]

To derive an expression for the generation rate due to sun illumination, we can go back to the hypothesis for this formulation. For a solar cell body being illuminated at area \(A\) and with the assumption that every incident photon generates an electron-hole pair, the generation rate from the solar illumination can be calculated in terms of the number of photons which have more energy than the bandgap.

\[
G_S(E) = A \int_{E_g}^{\infty} \frac{\lambda}{h c} S(E)dE \quad \text{with Bandgap } E_g = \frac{h c}{\lambda_g} \tag{2.10}
\]

where \(S(\lambda)\) is the spectral density of the incident light (e.g. AM 0 or AM 1.5). By considering a unit area of illumination and expressing it in terms of the wavelength, we obtain

\[
G_S(\lambda) = \int_{-\infty}^{\lambda_g} \frac{\lambda}{h c} S(\lambda)d\lambda \quad \text{where } \lambda_g = \frac{h c}{E_g} \tag{2.11}
\]

For a steady-state current-voltage relationship, the algebraic sum of the five processes mentioned earlier is zero.

\[
G_S - R_R + G_{NR} - R_{NR} - I/q = 0 \tag{2.12}
\]

\[
G_S - R_{R0} + (R_{R0} - R_R + G_{NR} - R_{NR}) - I/q = 0 \tag{2.13}
\]

It can be noted from Eq. 2.13 that the quantities inside the brackets are the net generation and recombination in the solar cell when it is surrounded by a blackbody of its own temperature. In order to formulate the current voltage relationship of the solar cells, the term \(f_R\) is introduced, which is defined as the fraction of generation-recombination current which is radiative. i.e.

\[
f_R = \frac{R_{R0} - R_R}{R_{R0} - R_R + G_{NR} - R_{NR}} \tag{2.14}
\]

Thus, we can obtain an equation for the current in the solar cell from Eqs. 2.13 and 2.14 as

\[
I(V, E) = q \left[ G_S - R_{R0} + (R_{R0} - R_R + G_{NR} - R_{NR}) \right] \tag{2.15}
\]

\[
I(V, E) = q (G_S - R_{R0}) + q \left( \frac{R_{R0} - R_R}{f_R} \right) \tag{2.16}
\]
As formulated by Shockley and Queisser, when we consider the only recombination process to be radiative, then \( f_R = 1 \), and from Eq. 2.16 we get

\[
I(V, E) = q(G_S - R_R)
\]  

where \( G_S \) and \( R_R \) are defined in Eqs. 2.11 and 2.9, which are dependent on the bandgap of the material and external voltage of the solar cell. Eq. 2.17 basically tells us that all the generated electron-hole pairs which do not recombine are contributing towards the current density. By setting the conditions \((V = 0)\) and \((I = 0)\), the short circuit current and open circuit voltage for the solar cell can be calculated from Eq. 2.17, respectively.

\[
I_{SC}(E) = q(G_S - R_{R0}) \quad \text{and} \quad V_{OC}(E) = \log\left(\frac{G_S}{R_{R0}}\right) \frac{kT_e}{q}
\]

In Fig. 2.3(b) and 2.3(c), the short circuit current and open circuit voltage as a function of the bandgap of the material is shown for illumination under AM 0 and AM 1.5 sun spectra. It is not surprising to see that as the band gap increases, the short circuit current decreases. Lesser photons have the energy required to generate electron-hole pair as the band gap increases. Also, since the irradiance of AM 0 is higher than AM 1.5 sun spectra, a higher short circuit current value for AM 0 illumination is obtained. The relationship of \( V_{OC} \) with bandgap shows that it behaves opposite to what is observed for the short circuit current. Shockley and Queisser have also shown that as the temperature of the solar cell \( T_c \to 0 \), the maximum value of \( V_{OC} \to V_g \), where \( V_g = \frac{E_g}{q} \) is the energy gap in volts. This property is also of importance since this mismatch of the \( V_{OC} \) and \( V_g \) contributes also to a fundamental loss in the solar cell.

So far, we have derived the current-voltage relationship of the solar cell in Eq. 2.17 and the quantities of \( I_{SC} \) and \( V_{OC} \) in Eqs. 2.18 and 2.19. These three equations are sufficient to calculate the fill factor and efficiency of the p-n junction solar cell as a function of the bandgap of the material.

\[
FF(E) = \frac{\max [qV_b(G_S - R_{R0})]}{I_{SC}(E)V_{OC}(E)} \quad \text{and} \quad \eta_{SQ}(E) = \frac{\max [qV_b(G_S - R_{R0})]}{P_{IN}}
\]

where \( V_b \) is the applied bias to the solar cell. The fill factor as a function of the bandgap is shown in Fig. 2.3(d). The maximum efficiency of a solar cell \( \eta_{SQ} \), considering only radiative recombination losses, is shown in Fig. 2.4. The maximum efficiency curves in Fig. 2.4 is shown for sun illumination AM 0 and AM 1.5. The calculated
Figure 2.3: (a) Spectral distribution of incident sunlight, case AM 0 and AM 1.5. Also shown are the different characteristic parameters of a solar cell as a function of the bandgap of the single junction solar cell material - (b) Short circuit current, (c) Open circuit voltage and (d) Fill factor.
Figure 2.4: Upper limit of efficiency for single junction solar cells as a function of the bandgap energy under AM 0 and AM 1.5 illumination. The yellow boxes indicate the maximum stabilized lab efficiencies of solar cells with the maximum achieved efficiency values denoted next to each box. The efficiency values were taken from the table published in Ref. [23].

efficiency curves are consistent with data published in Refs. [20, 22]. It has be noted that even though the efficiency of the solar cells under AM 1.5 illumination is higher, the amount of power on the incident light is higher under AM 0 illumination (1.353 kW/m² compared to 1 kW/m² for AM 1.5). Thus higher efficiency will not directly translate to higher absolute conversion efficiency towards power (in Watts) when the incident spectrum is changed. The bandgap of the commonly used materials for solar cell applications are also highlighted in Fig. 2.4. Silicon based solar cells and GaAs or CdTe based solar cells, they all are from the plateau region of the solar cell efficiency curve. The current efficiency limits of single junction solar cells based on the various materials are illustrated in the figure with the yellow boxes with their corresponding record efficiencies written next to each box. All these values were taken from the efficiency tables published in Ref. [23].

Along with the formulation of the maximum efficiency curve, the Shockley-Queisser limit also enables us to look into the fundamental losses which occur in a single junction solar cell. The efficiency of the solar cell is the available electric power from the solar cell. It is shown in the red area in Fig. 2.5. Along with it the loss due to the optical transparency of the material for incident photon with lesser energy than the bandgap of the material is shown in the green area of Fig. 2.5. According to the hypothesis,
only one electron-hole pair is generated from the incident photons with energy higher than the bandgap, thus the excess energy from the photon are also not properly utilized and contribute to thermalisation loss from the solar cell (illustrated with the blue area). The other losses, which are unavoidable due to the recombination of the photo-generated carriers and finite temperature of the solar cell (which lowers the \( V_{OC} \) to values lower than \( E_g \) (in Volts)), are shown in the gray area which sums up the entire contribution from the incident light to 100%. These fundamental losses calculated are consistent with various work from different groups in literature [16, 24, 25]. The Shockley-Queisser limit, of course, only considered the recombination losses. Detailed breakdown of all the possible fundamental losses in a single junction solar cell have been analyzed by Hirst and Ekins-Daukes in their work in Ref [25].

### 2.2 Thin-film silicon solar cells

Classical crystalline silicon solar cells consist of a p-n junction created from a p-type and an n-type domain formed within the same material. But solar cells based on amorphous and microcrystalline silicon materials can not be constructed by merely stacking a p-type and an n-type thin-film. Due to the very short lifetime of the photogenerated free charge carriers in the doped silicon layers, only a small fraction of the electron-hole pairs can be separated [26]. Thus, the stacked device will not show any photovoltaic activity. The short lifetime is the result of the high concentration of defects associated
2.2. Thin-film silicon solar cells

with p- or n-type doping of the material [26, 27]. Thus, in between the p- and n-type layers, an undoped layer with low defect density must be incorporated such that the photogenerated electrons in the intrinsic layer can be spatially separated and collected [28]. That is why in thin-film silicon solar cells based either on amorphous or microcrystalline single junction or their tandem, the intrinsic i-layer is sandwiched between the p- and n-type layers which generate the electric field.

Depending on the technology, solar cells can be deposited in either the superstrate or substrate form. The schematic structures of single junction and tandem silicon solar cells in superstrate configuration (p-i-n) are shown in Fig. 2.6. In superstrate configuration the incident light passes through the glass substrate before it enters the p-i-n solar cell. In substrate configuration, the deposition order is reversed, thus making the solar cell a n-i-p cell. In this configuration, the light directly enters the solar cell stack or in case of an encapsulated solar cell it enters through the encapsulation layer. The front contact of the solar cell consists of a transparent conductive oxide (TCO) layer - which is usually a film of aluminum doped zinc-oxide (ZnO:Al) or indium tin oxide (In$_2$O$_3$:SnO$_2$ or ITO). In practice, the TCO layer is also textured in order to enhance the optical performance of the device. Texturing allows the incident light to complete multiple passes within the thin absorber layer. Schematic of such textured solar cells are also shown in Fig. 2.6. The TCO layer is followed by the p-i-n diode(single junction)/p-i-n-p-i-n diode(tandem) layers. Since the layers are very thin, the texturing propagates all the way through to the back of the solar cell. Finally as back contact, either a single layer of silver (Ag) or a bi-layer of TCO/Ag or TCO/white paint is deposited to form the other contact of the solar cell.

With regards to the thicknesses for the individual layers, the TCO layer should be around 500 nm since it needs to allow for a sufficient lateral conductivity of the front electrode [29]. The doped silicon layers (p- and n-), on the other hand, are kept as thin as possible - usually in the range of 10-30 nm. Because of the poor electronic properties of the doped amorphous and microcrystalline silicon layers, most of the photogenerated electron-hole pairs in the doped layers do not contribute to the photo-current generated from the solar cell. The intrinsic silicon layer, where the electron-hole pairs are generated, should be thick enough such that it can utilize the incident optical spectrum. For amorphous silicon solar cells, the thickness of the absorber layer cannot be too large since it suffers from light induced degradation or as it is commonly known, due to Staebler-Wronski effect [30]. Due to the Staebler-Wronski effect, amorphous silicon under illumination creates additional defects in the band gap acting as recombination centers for photogenerated carriers, which in turn deteriorates its electrical properties.

In order to improve the light stability of amorphous silicon solar cells, the concept of tandem cells have been successfully applied to amorphous and microcrystalline silicon
Figure 2.6: Schematic device structures of single junction p-i-n solar cells and micromorph (amorphous and microcrystalline silicon) tandem cells in the ‘superstrate’ configuration. Solar cells deposited on smooth and textured TCO substrates are shown.

Moreover, it leads to better absorption of the sun spectrum as well. By utilizing a top cell from a very thin amorphous silicon p-i-n diode (i-layer thickness of around 200 nm), the amorphous silicon i-layer does not suffer further from Staebler-Wronski effect. Following the amorphous silicon p-i-n diode, the bottom cell consists of a microcrystalline silicon p-i-n diode which absorbs the longer wavelengths of the sun spectrum. Schematic of the micromorph (amorphous and microcrystalline silicon) tandem cell is shown in Fig. 2.6. This device structure is also advantageous since the open-circuit voltage is also increased. However, since the two p-i-n diodes are connected in series, the overall current flowing through the device is limited by the less current generating diode. Thus, in designing tandem solar cells, it is important to match the two diodes in a way, such that both the diodes can generate similar or almost similar photo-currents. This matching of the thicknesses of the top and bottom cells is generally referred to as current matching [33].

The p-i-n Solar Cell

A schematic sketch of a single junction p-i-n silicon solar cell and the electron-hole generation and separation inside the diode are shown in Fig. 2.7. A transparent conductive oxide and metal contact form the front and back contact of this device. The p- and n- layers (typical thickness of 10-30 nm) build up an electric field, which is ex-
Figure 2.7: Schematic sketch of a p-i-n solar cell. The charge separation of the electron-hole pairs are shown in the band diagram of the semiconductor device.

tended by inserting an intrinsic i-layer of silicon. Inside the i-layer, for each absorbed photon with energy higher than the silicon bandgap (1.1 eV for µc-Si and 1.7 eV for a-Si) an electron-hole pair is generated. By means of the electric field, these electrons and holes are then driven to the n- and p- layers, respectively. The diffusion lengths of the charge carriers in the intrinsic a-Si:H and µc-Si:H are typically 100 nm [33] and 200 nm [34] only. Since their diffusion length of the charge carriers are much smaller than the i-layer thickness, the extraction from the p-i-n diode results mainly from the drift of the electric field. Contrary to diffusion based crystalline silicon solar cells, the charge extraction in thin-film silicon solar cells is dictated by the electric field. Therefore thin-film silicon solar cells are also called drift cells.

The transport of the photogenerated carriers in a drift based p-i-n solar cell can be understood from the electron and hole continuity equations. There have been several publications in the early 1980s where the authors have derived and modeled the transport mechanism in a-Si based p-i-n solar cells [35–38]. Several authors have proposed the role of mobility×lifetime product, $\mu_T$, in order to evaluate the material property and performance of p-i-n solar cells [39, 40]. But as Shah et al. have noted in their work [41]: if in an actual p-i-n solar cell, the effective mobility×lifetime product were as high as those reported in various measurements [40, 42], it would have been feasible to fabricate a-Si:H solar cells with thickness of the i-layer larger than 1 µm even for solar cells in the degraded state. In practice, however, the i-layer thickness of solar cells based on a-Si:H are kept lower than 400 nm. Because of the non-uniform electric field in the i-layer of the p-i-n solar cell, the collection of charges in actual a-Si:H solar cells is very poor [41]. This detrimental effect imposes an electrical limitation on the performance of p-i-n solar cells which limits the thickness of the i-layer.
A schematic representation of the electric field within the p-i-n thin-film a-Si:H solar cell is shown in Fig. 2.8. The deformation of the electric field within the i-layer occurs due to defect-rich regions at the two interfaces. The defects are positively \((D^+\)) and negatively \((D^-\)) charged near the \(p/i\) and \(i/n\) interface, respectively. These defects in p-i-n a-Si:H solar cells, which become more dominant in degraded state, are mainly caused by charged dangling bonds and bandtail states. If the thickness of the i-layer is too thick or the density of charged defects are high, the electric field is deformed and reduced [43]. This deformation is illustrated in Fig. 2.8 where with higher mobility \times lifetime product the deformation of the electric field is reduced. The non-uniformity in electric field is not a sole characteristic of a-Si:H solar cells, but is also present in solar cells based on \(\mu\)c-Si:H as well. The requirement on i-layer thickness for \(\mu\)c-Si:H solar cells, however, are not as stringent as it is for a-Si:H solar cells since \(\mu\)c-Si does not suffer so much from light induced degradation like a-Si. From the perspective of electrical limitation on the solar cell, i-layer of \(\mu\)c-Si:H solar cells can be thicker than couple of microns and still have sufficient collection efficiency. In practice, typical i-layer thickness of \(\mu\)c-Si:H solar cells are in the range of 1-3 \(\mu\)m.

2.3 Solar Cell Material Properties

Thin-film silicon solar cells comprises of layers of a-Si:H or \(\mu\)c-Si:H or both and the transparent conductive oxide at the front, which in most cases and within the scope of this thesis is aluminum doped zinc-oxide (ZnO:Al). Their optical properties with respect to the incident wavelength plays a crucial role in designing efficient solar cells. Each of these layers can be described optically with their complex refractive index, \(\tilde{n} = n + i\kappa\). Where the real part, \(n\), is the refractive index and the imaginary part, \(\kappa\), is
Figure 2.9: Comparison of the optical absorption coefficients of microcrystalline silicon (µc-Si:H) and amorphous silicon (a-Si:H). Also shown is the curve for single crystal silicon (c-Si) as a reference. The corresponding penetration depth for the materials are also highlighted on the right hand side axis. This figure is adapted from Fig. 2.2 in Ref. [44].

called the extinction coefficient. The absorption coefficient, \(\alpha [\text{cm}^{-1}]\), is directly related to the extinction coefficient as

\[
\alpha = \frac{4\pi \kappa}{\lambda} \tag{2.22}
\]

We briefly discuss the optical properties of the solar cell materials in this section.

### 2.3.1 Optical Properties of a-Si:H and µc-Si:H

The optical absorption coefficients of the absorber materials in thin-film silicon solar cells are shown in Fig. 2.9. Along with the curves for a-Si:H and µc-Si:H, the absorption coefficient for single crystal silicon (c-Si) is also depicted as a reference. On the right hand side of the axis, the penetration depth for each material as a function of the incident wavelength is also highlighted. The top of the x-axis is also shown in terms of the photon energy, where the band gaps of a-Si:H (1.7 eV) and µc-Si:H (1.1 eV) are also marked.

Due to the lack of long range order, the law of momentum conservation is relaxed in a-Si:H and as a result, a-Si:H acts like a direct semiconductor [26]. Therefore the absorption coefficient of the material is determined by the availability of electronic
states only [26, 45]. Generally, the absorption edge near the band gap of a direct semiconductor is more abrupt than indirect gap materials. But as we can see from Fig. 2.9 the absorption coefficient for a-Si:H is not zero below the optical band gap of around 1.7 eV. This is due to the band tail states for a-Si:H. The conduction and valence band tail states give rise to subbandgap absorptions, giving rise to an exponential relationship between the absorption coefficient and photon energy [26, 33]. This exponential region of the optical absorption spectrum in the range of 1.4 eV and 1.7 eV is called the ‘Urbach tail’. Despite this subbandgap absorption region, when used as the p-i-n diode in a solar cell, a-Si:H is almost non absorbing for the longer wavelength (λ > 800 nm) region. μc-Si:H, on the hand, has similar optical band gap and properties like the the indirect semiconductor c-Si. Thus solar cells based on μc-Si:H benefits from absorbing photon energies in range of 1.1 eV to 1.7 eV, where a-Si:H solar cells show no response. The concept of using a-Si:H and μc-Si:H in tandem solar cells is therefore very favorable since it can utilize a broader sun spectrum.

2.3.2 Optical Properties of ZnO:Al

In order to achieve sufficient conductivity in the transparent conductive layers of a solar cell, the zinc-oxide (ZnO) films can be doped with aluminum (Al), gallium (Ga), boron (B) etc. And depending on the concentration of the doped metals, the optical properties of the films also vary. Most commonly these films are doped with Al. The transmission, reflection and absorption measurements of a ZnO:Al film doped with 0.5 wt% Al is shown in Fig. 2.10. In order to highlight the influence of the doping concentration, the absorption curve for a similar film with 1 wt% Al doping is also overlaid in the figure. As we can observe in Fig. 2.10, ZnO:Al appears to be very transparent in the visible and near infrared part of the optical spectrum. This is because of the higher band gap of undoped zinc-oxide, which is around 3.4 eV [46]. The optical properties of ZnO:Al as a function of the wavelength can be divided into three regions.

Region 1

The band gap 3.4 eV of zinc-oxide corresponds to wavelength of 365 nm. Which means for incident light with energies higher than the band gap are completely absorbed in the ZnO:Al film. The reflection in this region of around 8% corresponds to the reflection from the air/glass/ZnO:Al/air interfaces. Thus for incident wavelengths below the band gap of the film, the transmission through ZnO:Al is almost zero. It should be noted, that depending on the doping concentration the optical band gap of ZnO:Al will also change (Burstein-Moss shift) [48–51]. If the doping concentration is increased, the optical band gap shifts towards the shorter wavelengths.
2.3. Solar Cell Material Properties

Figure 2.10: Optical properties - Transmission, Reflection and Absorption - of a ZnO:Al film (doped with 0.5 wt% Al) as a function of the wavelength. The absorption curve for a film with different doping concentration (1.0 wt% Al) is also shown for comparison. This figure is adapted from Fig. 2 in Ref. [47].

Region 2

Since the photon energy is smaller than the optical band gap, no fundamental absorption occurs in this region. Up to wavelength of 1000 nm, we observe an interference pattern for the transmission and reflection curves. This Fabry-Perot interference pattern is caused by reflections from the front and back interface of the ZnO:Al film. Moreover, in this region the loss due to free-carrier absorption is limited to only 1-2% which kicks in after 1000 nm [52].

Region 3

In this region, a steady decrease in the transmission curve is observed. Due to the free-carrier absorptions, the ZnO:Al films starts absorbing more with increasing wavelength. At even longer wavelengths the reflection increases as well. Due to the high carrier concentration \( n > 10^{20} \text{cm}^{-3} \) the electrons in the film behave like free electrons in metals \( n \approx 10^{22} \text{cm}^{-3} \). The optical behavior in this region can be explained using classical Drude theory. For free electrons in metals, the plasma wavelength can be expressed as [52, 53]

\[
\lambda_p = \frac{2\pi e}{\sqrt{\frac{\varepsilon_\infty \varepsilon_0 m^*}{N e^2}}}
\]  

(2.23)
where \( c \) is the speed of light, \( \varepsilon_\infty \) is the high frequency dielectric constant, \( \varepsilon_0 \) is the permittivity of free space, \( m^* \) is the electron effective mass, \( N \) is the electron concentration and \( e \) is the elementary charge. The highest absorption occurs when the incident wavelength is at resonance with the plasma wavelength. In Fig. 2.10 the absorption peak for doping concentration of 0.5 wt% occurs after wavelength 2000 nm which is highlighted in the graph as \( \lambda_p \). For wavelengths larger than \( \lambda_p \) the film becomes reflective [52], which is also visible in the figure. From the absorption curve for ZnO:Al film with 1 wt% doping concentration, we can observe that high doping levels result in an enhanced absorption and also a shift of the plasma wavelength towards shorter wavelength (consistent with Eq. 2.23).

### 2.4 Light Confinement in Thin-film Silicon Solar Cells

It is desirable that the absorber layer of a thin-film silicon solar cell be as thin as possible. It reduces deposition time, requires less material and the electrical properties of devices also deteriorates less. But as we have already seen in Fig. 2.9, the penetration depth of a-Si:H and \( \mu \)c-Si:H near their band edge is in the order of 80 microns and 900 microns respectively. Which results in only a small fraction of the longer wavelength light being absorbed in such thin (around 300 nm for a-Si:H and 1 \( \mu \)m for \( \mu \)c-Si:H) solar cells. Like a classical optimization problem - the optical absorption inside the diode layer, while keeping its thickness as thin as possible, needs to be maximized. The goal of creating an electrically thin but optically thick solar cell is achieved by texturing the interfaces of the stratified thin-film silicon solar cell. By having a textured interface, the transmitted and reflected light can propagate at angles larger than the escape cone and thus can be confined within the absorber layer to complete multiple passes until it is absorbed. A schematic sketch highlighting the enhanced optical path length is shown in Fig. 2.11. Solar cells with and without textured interfaces are shown. For a solar cell on a smooth substrate, absorption occurs only for specularly transmitted and reflected light. Whereas light can travel at oblique angles after diffraction due to the introduction of texturing. The confinement of light within a thin absorber layer is coined as “light trapping”.

For sputtered zinc-oxide substrates, the most common technique to achieve light trapping structure is by etching the substrate in a dilute acid (e.g. 0.5% HCl) [54]. Together with highly reflective back contacts, these textured TCO substrates are commonly used to realize efficient a-Si:H and \( \mu \)c-Si:H solar cells. Since the conformally deposited silicon diode layers are very thin, the texturing from the etched TCO substrate serves as a template which propagates all the way through to the back contact. Experimentally measured quantum efficiency of p-i-n a-Si:H and \( \mu \)c-Si:H solar cells deposited on such textured TCO substrates are shown in Fig. 2.12. The quantum efficiency plots
of the solar cells deposited on smooth substrates are also shown as a reference. For the longer wavelengths ($\lambda > 600$ nm) where the silicon materials are poor absorbers, the quantum efficiency can be significantly boosted by confining the incident light within the thin diode layers. The enhanced quantum efficiency due to texturing results into higher short circuit current of the solar cell. The interference pattern that is visible for the solar cells on smooth substrates due to coherent nature of the propagating light is smoothened out after texturing. Due to scattering at the interface, the propagation of light in textured solar cells is semi-coherent or almost incoherent due to its multi directional spreading [55]. Compared to the short circuit current value of 11.80 mA/cm$^2$ achieved for the 360 nm thick a-Si:H solar cell deposited on a smooth substrate, a gain of 27% is achieved for the textured a-Si:H solar cell [Fig. 2.12(a)]. This relative gain increases to almost 50% for the $1\mu$m thick $\mu$c-Si:H solar cell [Fig. 2.12(b)] where the short circuit current values for the solar cell on a smooth substrate and textured substrate are 15.55 mA/cm$^2$ and 23.20 mA/cm$^2$, respectively. Due to the smaller band gap for $\mu$c-Si:H, the potential of $\mu$c-Si:H solar cells for light trapping is higher than a-Si:H based solar cells. Therefore tuning of optimal light trapping structures that can enhance the absorption in $\mu$c-Si:H solar cells are fundamental in achieving highly efficient micromorph(a-Si:H and $\mu$c-Si:H) tandem solar cells. The focus of our study in this thesis is also based on optimizing the structures that are beneficial for $\mu$c-Si:H solar cells.
Textured TCO Substrates

In the previous discussion regarding textured ZnO:Al substrates, the roughening of the sputtered TCO substrates were done in a post deposition step. After the deposition of a smooth ZnO:Al film on a glass substrate, it was etched in a dilute acid in order to create texture etched substrate. By varying the concentration and type of the acid, the feature sizes of the textures on the surface can be tuned [57]. By depositing the film using low pressure chemical vapor deposition (LPCVD), similar textured TCO substrates can also be formed while the film is being grown [31]. In Fig. 2.13 atomic force microscopy of TCO substrates deposited using sputtering and LPCVD are shown. At the top row, 2-dimensional top view of the surfaces are shown and the corresponding 3-dimensional projections are shown just below each figure. As deposited smooth ZnO:Al film on a glass substrate is shown in Fig. 2.13(a). A smooth film is deposited with a surface RMS (root mean square) roughness of only 4.8 nm. When this smooth substrate was etched in a 0.5% HCl acid for 30 seconds, the resulting textured surface is shown in Fig. 2.13(b). The calculated RMS roughness for this surface profile was 43.5 nm. From the distribution of craters on its surface it is evident that the crater size and depth is indeed random. While there are some very deep craters, a large fraction of the surface are not too rough and have very shallow craters. The RMS roughness for the surface profile of the substrate deposited using LPCVD [Fig. 2.13(c)] was also in the same range for that from the texture etched substrate. It was calculated to be 48.6 nm. Despite this resemblance in their roughness, the shape of the texturing on the substrate is very different to the crater that is created after etching in dilute acid. The
2.4. Light Confinement in Thin-film Silicon Solar Cells

Figure 2.13: Atomic force microscopy images of (a, b) sputtered zinc-oxide substrates and deposited using (c) LPCVD (low pressure chemical vapor deposition). (a) Shows the surface profile of as deposited zinc-oxide substrate, and (b) shows the surface of a substrate etched in 0.5% HCl for 30 seconds. The RMS roughnesses ($\delta_{rms}$) were 4.8 nm, 43.5 nm and 48.6 nm, respectively.

shape can be attributed as upright pyramids with a small distribution in terms of its size. Most of the feature sizes have a base period typically close to 500 nm. It has been seen that substrates deposited using LPCVD are more suited for a-Si:H solar cells.

There are of course several other concepts where scientists have tried to achieve better light trapping performance than these above mentioned techniques. Commercially available Asahi-U tin-oxide ($\text{SnO}_2$:F) substrates deposited on soda-lime glass by using atmospheric pressure chemical vapor deposition (APCVD) have been the de facto standard for a-Si:H solar cells for very long [58, 59]. Asahi glass have proposed newer double texturing substrates, namely Asahi-W substrate in the recent years [60]. Such double textured substrates have also been reported by researchers at Tokyo Tech [61]. Recent publications have also reported fabricating the textured zinc oxide films from nanoimprint or by growing zinc oxide nanowires[62–65]. The transparent conductive oxide is an important piece of the puzzle which can unlock the gateway towards highly efficient thin-film silicon solar cells.

2.4.1 Light Trapping Limits

An ideal textured interface, which scatters all the light diffusively, will exhibit a lambertian scattering pattern. A lambertian pattern means that the ADF (angular distribution
function) of the transmission/reflection from a textured surface is determined by a cosine function \([66]\). And for such an ideal textured interface, the maximum enhancement in terms of the absorbed optical intensity was first derived by Yablonovitch and Cody in their work in 1982. Detailed description on the formulation is given by the authors in their paper in Ref. [67]. Yablonovitch and Cody derived, that for a weakly absorbing material slab, the effective absorption can be enhanced to as high as \(4n^2\) in a perfectly textured solar cell, where \(n\) is the real part of the complex refractive index of the material. With a typical refractive index of 3.50 this factor is around 50 for silicon. For an indirect band gap like silicon which absorbs very poorly near its band edge, a perfect light trapping structure can therefore enhance the absorption and make efficient utilization of the incident sunlight.

For a solar cell deposited on a smooth substrate (without texturing), the absorption in the slab \(A_{NoLT}\) can be calculated as

\[
A_{NoLT}(\lambda) = 1 - \exp \left[-2\alpha(\lambda) d\right]
\]

(2.24)

where \(\alpha(\lambda)\) is the absorption coefficient of the material as a function of the incident light and \(d\) is the thickness of the slab. This absorption only takes into account the double pass that happens due to the back reflector of the solar cell. In an idealized

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**Figure 2.14:** Maximum achievable absorption in silicon solar cells for different thicknesses of the absorber layer (1, 10 and 50 \(\mu m\)). Additional curve for a 1 \(\mu m\) thick solar cell with a perfect lambertian texturing is also shown to highlight the enhancement due to perfect light trapping.
2.4. Light Confinement in Thin-film Silicon Solar Cells

textured film, there should be multiple passes of light within the absorber layer such that the path lengths of the oblique rays are highly enhanced. Applying Yablonovitch and Cody’s enhancement factor for an idealized lambertian light trapping texture, the maximum absorption in a slab $A_{WLT}$ due to light trapping can be calculated as

$$A_{WLT} (\lambda) = 1 - \exp \left[ -4n^2 \alpha (\lambda) d \right]$$  \hspace{1cm} (2.25)

where $n$ is the real part of the complex refractive index of the material. The theoretically achievable absorptions (using Eq. 2.24) in silicon solar cells deposited on smooth substrates with varying thicknesses are shown in Fig. 2.14. With increasing absorber layer thicknesses from 1 $\mu$m, to 10 and 50 $\mu$m, we can observe that the absorption in the longer wavelengths, where silicon is a weak absorber, is enhanced due to higher optical path lengths of the incident photons. The total short circuit current increases from 18.33 mA/cm$^2$ to 33 and 38.7 mA/cm$^2$ for these three cases with increasing thicknesses. Similar effect of enhanced absorption in the longer wavelengths is achieved by applying the lambertian texturing condition to even the thinnest solar cell with absorber of 1 $\mu$m only. The absorption curve (using Eq. 2.25) for such a case which enhances the optical path length of the photons near the band edge of silicon to $4n^2$ is also shown in Fig. 2.14. Compared to the solar cell on a smooth substrate, the textured solar cell exhibits an enhancement of 18.4 mA/cm$^2$. 
Chapter 3

Computational Modeling of Optical Wave Propagation

Light propagates as an electromagnetic wave, whose properties are governed by the Maxwell’s equations. By formulating the set of four equations, James Clerk Maxwell established, for the first time, the bilateral relationship between electricity and magnetism.\(^1\) With the advent of computers, the capability of scientists and engineers to solve Maxwell’s equations for real world applications has changed profoundly. Before mid-1960s when modern digital computers were not available, most electromagnetic problems were solved using analytical methods such as separation of variables, series expansion etc. While these methods were useful for smaller idealized structures, for realistic problems it meant approximation and simplification of the problem. Consequently it resulted in solutions with lower accuracy. Nowadays with the ever increasing processing capabilities of computers, solution of the Maxwell’s equations for complex geometries is possible even with our home personal computers. Several methods exist to solve the electromagnetics problem numerically. There is of course no one single best method which can solve the numerical problem with high precision and also using lower computation power. In this chapter, we briefly describe the computation algorithms used to investigate the optical wave propagation in a thin-film silicon solar cell.

3.1 Optics in Textured Interfaces

The device structure of thin-film silicon solar cells deposited on a smooth substrate can be described as a stack of stratified homogeneous layers. In order to model the light propagation or calculating the absorption in such nanostructured devices, using modeling tools that solves the Maxwell’s equations rigorously is not necessary - simple

\(^1\)James Clerk Maxwell (1831-1879) published the set of four equations in his paper titled *A Dynamical Theory of the Electromagnetic Field* (1865).
calculations using transfer matrix method would suffice \[68\]. Applications of transfer matrix method is seen in designing anti-reflection coatings, beamsplitters, dielectric filters etc. But as described in the previous chapter, thin-film silicon solar cells are rarely deposited on a smooth substrate. In order to increase the optical path length of light within the absorber layer, textured interfaces are utilized.

It is well known that the interplay between size of the texturing and wavelength of the incident light defines the behavior of the optical propagation in that system. The transmission, reflection and absorption of light in the system can be tuned by varying these two parameters. Different theories can be used to describe the optical behavior of light in these different circumstances where the period of the texturing is either:

1. Very small compared to the incident wavelength.
2. Comparable to the incident wavelength.
3. Much larger than the incident wavelength.

An illustration of these three cases is shown in Fig. 3.1. For example, in case of Fig. 3.1(a), the feature size of the texture is much smaller than the incident wavelength. In such a system the light propagation can be explained using the effective medium theory (EMT). By applying effective medium theory to a spatially varying interface between two materials, the textured region is substituted with an “effective” material with homogeneous properties \[69\]. And if it’s the other way around like the case in Fig. 3.1(c), where the feature sizes are much larger than the wavelength - scalar theory or geometric optics can be used. But in both these two cases, majority of the light is either transmitted through or reflected back. Hence, for enhanced light trapping in thin-film solar cells we require interfaces with texture period in the range of the wavelength of light. Because in such an arrangement, we can expect to obtain the diffracted and scattered light inside the silicon absorber that can contribute to higher efficiency of the solar cell.

The textured interfaces used for enhanced light trapping in thin-film silicon solar cells consist of wavelength-scale features. In sputtered zinc oxide with post-deposition wet etching, as grown zinc oxide from low pressure chemical vapor deposition (LPCVD) or in commercially available tin oxide substrates (Asahi-U): the feature sizes in these textured substrates all have periods in the range of the incident wavelength. Since optics plays a major role for achieving higher efficiencies in thin-film silicon solar cells, understanding of the optical wave propagation in these nanostructured devices are crucial in finding the optimized device structure. However, complete optical description of light propagation inside the layers of thin-film solar cells with such feature sizes (case in Fig. 3.1(b)) cannot be explained using simple scalar theories of light. When the scale of the feature sizes are in the same order as the illumination wavelength, only
3.2. Review of Electromagnetics Theory

The properties of electromagnetic fields in a medium unfolds as a logical deduction from the four Maxwell’s equations [70]. We start with the set of four Maxwell’s equations. These equations connect the five basic quantities $E$ (electric field intensity), $H$ (magnetic field intensity), $B$ (magnetic flux density), $D$ (electric flux density) and $J$ (current density).

$$\nabla \times E + \frac{\partial B}{\partial t} = 0$$ \hspace{1cm} (3.1)

$$\nabla \times H - \frac{\partial D}{\partial t} = J$$ \hspace{1cm} (3.2)

$$\nabla \cdot D = \rho$$ \hspace{1cm} (3.3)

$$\nabla \cdot B = 0$$ \hspace{1cm} (3.4)

where $\rho$ is the electric charge density. $E$ and $D$ are the electric field quantities; $B$ and $H$ are the magnetic field quantities which are interrelated by the following constitutive relations.

**Figure 3.1:** Relationship between the period of a textured substrate and the incident wavelength. The wave propagation in the optical systems with different feature sizes of the texture can be explained by (a) effective medium theory, (b) rigorously solving the Maxwell’s equations and (c) scalar theory or geometric optics.
with $\epsilon$ being the electrical permittivity of the material and $\mu$ being the magnetic permeability of the material. These equations hold in any material, including free space and at any spatial location.

**Wave Equation**

A necessary condition for $\mathbf{E}$ and $\mathbf{H}$ to satisfy the Maxwell’s equations is that each of their components can satisfy the wave equation [71]. In order to obtain the equation, we can start with either of the Maxwell’s curl equations (3.1) or (3.2). Here we start with equation 3.1. For a linear isotropic, homogeneous and source-free medium ($\rho = 0, \mathbf{J} = 0$), taking the curl of both sides of equation 3.1 and using the relationship from equation 3.6 gives

$$\nabla \times \nabla \times \mathbf{E} = -\mu \frac{\partial}{\partial t} (\nabla \times \mathbf{H})$$

(3.7)

since $\mathbf{J} = 0$, by using the relationships from equation 3.2 and 3.5, equation 3.7 becomes

$$\nabla \times \nabla \times \mathbf{E} = -\mu \epsilon \frac{\partial^2 \mathbf{E}}{\partial t^2}$$

(3.8)

Applying the vector identity $\nabla \times \nabla \times \mathbf{A} = \nabla (\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A}$ to equation 3.8, we get

$$\nabla (\nabla \cdot \mathbf{E}) - \nabla^2 \mathbf{E} = -\mu \epsilon \frac{\partial^2 \mathbf{E}}{\partial t^2}$$

(3.9)

since $\rho = 0$, from equations 3.3 and 3.5 we get that $\nabla \cdot \mathbf{E} = 0$, and hence we obtain

$$\nabla^2 \mathbf{E} - \mu \epsilon \frac{\partial^2 \mathbf{E}}{\partial t^2} = 0$$

(3.10)

which is the time-dependent vector Helmholtz equation or simply wave equation. If we had started the derivation with equation 3.2, we would have obtained the wave equation for $\mathbf{H}$ as

$$\nabla^2 \mathbf{H} - \mu \epsilon \frac{\partial^2 \mathbf{H}}{\partial t^2} = 0$$

(3.11)

These two equations (3.10) and (3.11) are equations of motion of electromagnetic waves that travel in a medium with a velocity of

$$\nu = \frac{1}{\sqrt{\mu \epsilon}}$$

(3.12)
In free space, with electromagnetics constants \( \mu_0 = 4\pi \times 10^{-7} \text{ H/m} \) and \( \epsilon_0 = 8.854 \times 10^{-12} \text{ F/m} \), we obtain the speed of light \( \nu = c \approx 3 \times 10^8 \text{ m/s} \).

**Optical Intensity and Power**

In electromagnetic theory light intensity is interpreted as the energy flux of the electric field. The energy law of electromagnetic fields can be derived from the time dependent Maxwell’s curl equations (3.1) and (3.2). By scalar multiplication of \( \mathbf{H} \) and \( \mathbf{E} \) with equations (3.1) and (3.2) respectively, we obtain

\[
\mathbf{H} \cdot (\nabla \times \mathbf{E}) = -\mathbf{H} \cdot \frac{\partial \mathbf{B}}{\partial t} \quad (3.13)
\]

\[
\mathbf{E} \cdot (\nabla \times \mathbf{H}) = \mathbf{E} \cdot \mathbf{J} + \mathbf{E} \cdot \frac{\partial \mathbf{D}}{\partial t} \quad (3.14)
\]

subtracting equation (3.14) from equation (3.13) yields

\[
\mathbf{H} \cdot (\nabla \times \mathbf{E}) - \mathbf{E} \cdot (\nabla \times \mathbf{H}) = -\mathbf{H} \cdot \frac{\partial \mathbf{B}}{\partial t} - \mathbf{E} \cdot \frac{\partial \mathbf{D}}{\partial t} \quad (3.15)
\]

Using the vector identity \( \nabla \cdot (\mathbf{A} \times \mathbf{B}) = \mathbf{B} \cdot (\nabla \times \mathbf{A}) - \mathbf{A} \cdot (\nabla \times \mathbf{B}) \), the left hand side of equation (3.15) can be deduced resulting in the following

\[
\nabla \cdot (\mathbf{E} \times \mathbf{H}) = -\mathbf{H} \cdot \frac{\partial \mathbf{B}}{\partial t} - \mathbf{E} \cdot \frac{\partial \mathbf{D}}{\partial t} - \mathbf{E} \cdot \mathbf{J} \quad (3.16)
\]

For bodies at rest and isotropic materials, the medium dependent equations are \( \mathbf{D} = \epsilon \mathbf{E} \), \( \mathbf{B} = \mu \mathbf{H} \) and \( \mathbf{J} = \sigma \mathbf{E} \), where \( \sigma \) is the conductivity of the material. Utilizing these three relations, the expressions on the right hand side of equation (3.16) can be rewritten as

\[
\mathbf{H} \cdot \frac{\partial \mathbf{B}}{\partial t} = \mu \left( \mathbf{H} \cdot \frac{\partial \mathbf{H}}{\partial t} \right) = \mu \frac{1}{2} \frac{\partial}{\partial t} (\mathbf{H} \cdot \mathbf{H}) = \frac{\partial}{\partial t} \left( \frac{1}{2} \mu \mathbf{H}^2 \right)
\]

\[
\mathbf{E} \cdot \frac{\partial \mathbf{D}}{\partial t} = \epsilon \left( \mathbf{E} \cdot \frac{\partial \mathbf{E}}{\partial t} \right) = \epsilon \frac{1}{2} \frac{\partial}{\partial t} (\mathbf{E} \cdot \mathbf{E}) = \frac{\partial}{\partial t} \left( \frac{1}{2} \epsilon \mathbf{E}^2 \right)
\]

\[
\mathbf{E} \cdot \mathbf{J} = \sigma (\mathbf{E} \cdot \mathbf{E}) = \sigma \mathbf{E}^2
\]

inserting these expressions back into equation (3.16) gives

\[
\nabla \cdot (\mathbf{E} \times \mathbf{H}) = -\frac{\partial}{\partial t} \left( \frac{1}{2} \epsilon \mathbf{E}^2 + \frac{1}{2} \mu \mathbf{H}^2 \right) - \sigma \mathbf{E}^2 \quad (3.17)
\]

Integrating equation (3.17) throughout an arbitrary volume \( V \) (enclosed by a surface \( S \)) and then applying Gauss’s divergence theorem\(^2\) yields

\[^2\text{The divergence theorem relates the volume integral of } \nabla \cdot \mathbf{F} \text{ over any volume } V \text{ to the flux of } \mathbf{F} \text{ through the closed surface } S \text{ that bounds } V. \text{ That is, } \int_V \nabla \cdot \mathbf{F} \, dv = \oint_S \mathbf{F} \cdot ds\]

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3. Computation Modeling of Optical Wave Propagation

\[ \oint_{Vol} \nabla \cdot (E \times H) \, dv = \oint_{Vol} \left\{ -\frac{\partial}{\partial t} \left( \frac{1}{2} \epsilon E^2 + \frac{1}{2} \mu H^2 \right) - \sigma E^2 \right\} \, dv \]  
\[ (3.18) \]

\[ \oint_S (E \times H) \cdot ds = -\frac{\partial}{\partial t} \oint_{Vol} \left( \frac{1}{2} \epsilon E^2 + \frac{1}{2} \mu H^2 \right) \, dv - \oint_{Vol} (\sigma E^2) \, dv \]  
\[ (3.19) \]

Equation (3.19) establishes the conservation of energy in electromagnetics and is also known as the Poynting theorem. It states that the power flow out of the surface \( S \) equals to the decreasing rate of the stored electric and magnetic energies plus the power supplied by the source. The quantity on the left hand side of equation is defined as the Poynting vector. For an electromagnetic wave with an electric field \( E \) and magnetic field \( H \), the Poynting vector \( S \) is defined as

\[ S = E \times H \]  
\[ (3.20) \]

\( S \) represents the power per unit area (power density) carried by the wave and its direction is along the propagation direction of the wave. In practice, however, the quantity of greater interest is the average power density of the wave. For example in optics, when one refers to the amount of light illuminating a surface, it refers to the average energy per unit area per unit time - called the irradiance \( (I) \). The time-average value of the magnitude of \( S \) is a measure of \( I \) \( (I \equiv \langle S \rangle_T) \). In the case of a harmonic and linearly polarized plane wave traveling through free space, irradiance is proportional to the square of the amplitude of the electric field.

\[ I \equiv \langle S \rangle_T = \frac{1}{2} c \epsilon_0 E^2 \]  
\[ (3.21) \]

where \( c \) is the speed of light and \( \epsilon_0 \) is the electric permittivity of free space. It can be noted from equation (3.21) that since \( I \) depends only on the magnitude of the electric field, waves characterized by different polarization of light carry the same amount of average power if their electric fields have the same magnitude. In this section, a very brief review from the theories of electromagnetics were presented. Detailed description on the topic can be found in several textbooks where it is discussed in depth, interested readers are recommended to check references [68, 70–73].

3.3 Maxwell’s Equations Solver

Although the most accurate result for an electromagnetic field problem can be achieved using mathematical analytical method, most of real-life electromagnetics problems
deal with cases: where the system is described as non-linear PDE (partial differential equation), the boundary conditions are of mixed type, the solution region is complex etc. And to solve such problems with higher complexities, it is imperative to use numerical methods. There exist different algorithms that are used in solving such problems. Most widely used are finite difference method (FDM), finite element method (FEM) and method of moments (MoM) [70].

In finite difference methods, the differential forms of Maxwell’s equations are discretized - replacing the differential equations by finite difference equations. Among finite difference methods, most commonly used is its time domain difference, namely finite difference time domain method (FDTD). FDTD is a very efficient method which requires fewer grid operations. Integral form of Maxwell’s equations can also be discretized, these methods include method of moments (MoM) and finite integration technique (FIT). MoM is advantageous for problems involving open regions, and when the current carrying surfaces are small; this method is also often applied to scattering problems [74]. The other method that divides the computational region into unstructured grids (typically into triangles) is called finite element method (FEM). Even though methods based on FDM and MoM are conceptually simpler and easier to program, the major advantage of FEM lies in its versatility in numerical modeling of structures involving complex and large geometries and inhomogeneous media [70].

Since, in this study, a FDTD based software was used to investigate the optical wave propagation in thin-film silicon solar cells, only a brief introduction to this method is presented here in this section. For more information regarding the other fullwave electromagnetics solvers, the readers are suggested to refer to references [70, 74]. FDTD is one of the most popular computational methods for microwave problems; it is simple to program, highly efficient, and easily adapted to deal with a variety of problems. A major weakness of the FDTD algorithm lies in the way it deals with boundaries that are not aligned with the cartesian grid: for oblique boundaries, FDTD programs uses a kind of “staircase approximation”. But on the other hand due to its explicit nature, FDTD does not require inversion of matrices in its calculation and thus there is no limit to the size of the computational domain rather only the time required by the computer is FDTD’s computational limitation [75].

In terms of numerically solving the Maxwell’s equations, there also exists a class of algorithms that are well suited for infinitely periodic structures. If the precondition of a periodic surface is fulfilled, modal method (MM) [76], C-method [77] or rigorous coupled-wave analysis (RCWA) methods [78] also provide an accurate and computationally less demanding solutions (compared to FDTD, FEM etc.) to electromagnetics problems. Within the scope of this thesis work, since periodically textured structures have been extensively investigated, along with the results presented from FDTD solvers, we also discuss results obtained from rigorous coupled-wave analysis
method. In the following, we briefly describe the working principle of FDTD and RCWA algorithms.

### 3.3.1 Finite Difference Time Domain Method

The finite difference time domain method, first introduced by Kane S. Yee [79] in 1966 is a direct solution of the Maxwell’s time dependent curl equations (3.1) and (3.2). In an isotropic medium, these equations can also be written as

\[
\frac{\partial H}{\partial t} = -\nabla \times E \tag{3.22}
\]

\[
\epsilon \frac{\partial E}{\partial t} + \sigma E = \nabla \times H \tag{3.23}
\]

By expanding these equations for a rectangular coordinate system, we obtain

\[
\frac{\partial H_x}{\partial t} = \left( \frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} \right) \tag{3.24}
\]

\[
\frac{\partial H_y}{\partial t} = \left( \frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} \right) \tag{3.25}
\]

\[
\frac{\partial H_z}{\partial t} = \left( \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} \right) \tag{3.26}
\]

\[
\epsilon \frac{\partial E_x}{\partial t} + \sigma E_x = \left( \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} \right) \tag{3.27}
\]

\[
\epsilon \frac{\partial E_y}{\partial t} + \sigma E_y = \left( \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} \right) \tag{3.28}
\]

\[
\epsilon \frac{\partial E_z}{\partial t} + \sigma E_z = \left( \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \right) \tag{3.29}
\]

Following Yee’s notations, these set of 6 equations can be discretized with central finite difference approximation as long as they lie on a staggered grid. The simulation domain of the cubic box is called the Yee cell. In the Yee’s cell scheme, the \(E\) and \(H\) fields for each grid point are arranged specially. The electric field components are computed at “integer” time-steps and the magnetic field at “half-integer” time-steps. And space is divided into blocks with \(\Delta x\), \(\Delta y\), and \(\Delta z\) discretization. The different field components are placed in the grid according to the unit cell shown in Fig. 3.2.

Expanding equation (3.24) in terms of central finite difference, we can obtain explicit finite difference approximation as

\[
\frac{H_x^{n+1/2}(i, j, k) - H_x^{n-1/2}(i, j, k)}{\Delta t} = \frac{E_y^n(i, j, k) - E_y^n(i, j, k - 1)}{\Delta z} - \frac{E_z^n(i, j, k) - E_z^n(i, j - 1, k)}{\Delta y}
\]

Solving for \(H_x^{n+1/2}(i, j, k)\), we have
Figure 3.2: Unit cell of the Yee’s lattice. The positions and directions of the electric and magnetic field components are highlighted as well.

\[ H_{x}^{n+1/2}(i, j, k) = \frac{\Delta t}{\mu \Delta z} \left( E_{y}^{n}(i, j, k) - E_{y}^{n}(i, j, k - 1) \right) \]
\[ - \frac{\Delta t}{\mu \Delta y} \left( E_{z}^{n}(i, j, k) - E_{z}^{n}(i, j - 1, k) \right) + H_{x}^{n-1/2}(i, j, k) \] (3.30)

Similar procedure can be applied to equations (3.25) and (3.26), and we can derive the explicit finite difference equations for the other 2 components of H.

\[ H_{y}^{n+1/2}(i, j, k) = \frac{\Delta t}{\mu \Delta x} \left( E_{y}^{n}(i, j, k) - E_{y}^{n}(i - 1, j, k) \right) \]
\[ - \frac{\Delta t}{\mu \Delta y} \left( E_{x}^{n}(i, j, k) - E_{x}^{n}(i, j, k - 1) \right) + H_{y}^{n-1/2}(i, j, k) \] (3.31)

\[ H_{z}^{n+1/2}(i, j, k) = \frac{\Delta t}{\mu \Delta y} \left( E_{z}^{n}(i, j, k) - E_{z}^{n}(i, j, k) \right) \]
\[ - \frac{\Delta t}{\mu \Delta x} \left( E_{y}^{n}(i, j, k) - E_{y}^{n}(i - 1, j, k) \right) + H_{z}^{n-1/2}(i, j, k) \] (3.32)

Expanding equation (3.27) in terms of central finite difference, we can obtain explicit finite difference approximation for the electric field as
3. Computational Modeling of Optical Wave Propagation

The six equations (3.30)–(3.35) are the first order difference equations defining Yee's algorithm and the foundation of the FDTD method [79, 80]. It can be noted from equations (3.30) till (3.35) and from Fig. 3.2, that the components of \( E \) and \( H \) are interlaced within the unit cell and are evaluated at alternate half-time steps. Thus the FDTD algorithm is also called leap-frog algorithm. In such a configuration, in order to update the electric field components (\( E^n \)) the magnetic field components (\( H^{n-1/2} \)) calculated in the previous step are used, and the updated electric field components
3.3. Maxwell’s Equations Solver

Figure 3.3: Space time arrangement of the electric and magnetic field components with the leap-frog algorithm for wave propagation in a one-dimensional case. Initial conditions are set to zero for both the electric and magnetic field components.

\[(E^n)_n\text{ obtained are then used to update the next magnetic field components } (H^{n+1/2}).\text{ An illustration of the leap-frog scheme is shown in Fig. 3.3, where the wave propagation in a one-dimensional case is considered. In translating the system of equations from (3.30)-(3.35) into a computer code, it has to be noted, that within the same time loop one field component has to be calculated first and the results obtained are then used in calculating the other type [70]. In solving a electromagnetic field problem, the evolution of the electromagnetic fields are computed as follows}

1. Set initial conditions. (Usually let \(n = 0\), \(E^0 = 0\) and \(H^{-1/2} = 0\)).
2. Compute values for sources at \(n\).
3. Compute \(H^{n+1/2}\).
4. Compute \(E^{n+1}\).
5. Check for convergence of solution. If not finished then let \(n = n + 1\) and go to step 2.
6. Perform post processing.

**Stability of FDTD**

The fundamental constraint of FDTD method is the step size both for the time and space domains. Space and time steps relate to the accuracy, numerical dispersion, and the stability of the FDTD method. In order to ensure the accuracy of the computed results, the spatial increment or the mesh size should be 1/10 or less at the shortest wavelength [81]. Since FDTD is a volumetric computational method, when solving problems with dielectrics, there is a relation between the maximum grid size to the refractive index and the wavelength of the light. This permissible size is given by

\[
\text{Maximum grid size} = \text{minimum} (\Delta x, \Delta y, \Delta z) \leq \frac{\lambda_{\min}}{10n_{\max}} \quad (3.36)
\]
where $n_{\text{max}}$ is the maximum refractive index in the computational medium. Once the cell size is determined, the maximum time step is also limited by the following relationship [80, 82]

$$\text{Maximum time step} = \Delta t \leq \frac{1}{v \sqrt{\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} + \frac{1}{(\Delta z)^2}}}$$

(3.37)

where $v$ is the speed of light in the medium. Equation 3.37 defines the Courant-Fredrichs-Lewy (CFL) stability limit of the three-dimensional Yee’s algorithm for Maxwell’s equations [83, 84].

### 3.3.2 Rigorous Coupled-Wave Analysis

The rigorous coupled-wave analysis was first formulated by Moharam and Gaylord for planar one-dimensional gratings and was subsequently extended to surface relief gratings [85, 86]. Since this method is only applicable to periodic structures, the material structure and the electromagnetic fields in the system can be represented in terms of series expansions. In the coupled-wave representation, the fields inside the grating are expanded in terms of the space harmonics of the fields in the periodic structure. When the expansion is done in terms of the modes, then the method is called modal method. Even though there is this distinction in formulating the problem, both these methods have been shown to be giving equivalent results by Gaylord and Moharam [87].

Common to all modal and wave approaches, the dependence of the changing permittivity in the direction of the wave propagation is removed. A schematic of a grating
system typical to problems which use rigorous coupled-wave analysis is shown in Fig. 3.4. For such a grating configuration, the system can be divided into three regions. The incident medium is in Region 1 and the substrate is in Region 3. The intermediate Region 2 with the periodic grating structure is then approximated by slicing the grating region into a stack of L lamellar layers. By stratifying the grating region, the permittivity in each layer only changes periodically along the x-direction. This enables us to expand the relative permittivity in each layer as a Fourier series. If the individual layers are sufficiently thin, then the Fourier components of the complex relative permittivity are constant within each thin layer. For a thickness of the lth stratified layer $d_l$ in Region 2, the periodic relative permittivity is given by

$$
\epsilon_l(x) = \sum_m \epsilon_{l,m} \exp[j (2\pi m / \Lambda)], \text{ with } D_l = \sum_{p=1}^l d_p
$$

(3.38)

where $\epsilon_{l,m}$ is the mth Fourier component of the relative permittivity of the layer l. Then the diffraction problem of the multilayered system is solved in the following sequence of steps [78].

1. In each stratified grating layer, the coupled-wave equations are constructed and are solved for the electromagnetic fields.

2. The electromagnetic boundary conditions (continuity of the tangential electrical and magnetic field components) are applied between the Region 1 (input) and the first grating layer. Then between the first and second grating layers, and so forth, and finally between the last grating layer and Region 3 (output).

3. The resulting array of boundary condition equations is solved for the reflected and transmitted diffracted field amplitudes, and the diffraction efficiencies are determined.

Since we have not used RCWA very extensively in our work for this thesis, detailed formulation of the implementation for the RCWA algorithm is not being given here. But interested readers are recommended to read the research papers from the works of Moharam and Gaylord and their colleagues [85, 88].

**Acknowledgment**

The lecture notes from the graduate course “Computational Electromagnetics” offered at Jacobs University by Prof. Jon Wallace was of great help for the formulation of the FDTD algorithm.
Chapter 4

$c$-Si Solar Cells with Integrated Lamellar Gratings

The optics of microcrystalline silicon thin-film solar cells with integrated lamellar grating structures was investigated. Periodic grating couplers were integrated in microcrystalline silicon thin-film solar cells and the influence of the grating dimensions (grating period and grating height) on the short circuit current and the quantum efficiency was investigated. The grating structure leads to scattering and higher order diffraction resulting in an increased absorption of the incident light in the silicon thin-film solar cell. Enhanced quantum efficiencies are observed for the red and infrared parts of the optical spectrum. By investigating the influence of the front and back grating, optimal dimensions of the grating coupler were obtained.

4.1 Optical Simulation Model

In order to achieve higher short circuit current from microcrystalline silicon thin-film solar cells, the favored method in research labs and industry is by texturing the interfaces of the solar cells. The highest efficiencies of more than 10% have been achieved by the researchers at Kaneka Corporation [6] for 2 $\mu$m thick poly-Si solar cell using the STAR\textsuperscript{1} structure. Similar efficiencies, higher than 8%, have been reported by researchers at Research Center Jülich [89] and University of Neuchâtel [31] where they texture the transparent conductive oxide layer by wet etching of the deposited layer in a dilute HCl (hydrochloric acid) acid or by depositing the zinc oxide layer in a low pressure chemical vapor deposition process. Introducing nanotextured interfaces leads to enhanced scattering and diffraction of light in the device. Compared to that of a solar cell on a smooth surface, the optical path length is increased, which leads to a distinctly enhanced short circuit current and quantum efficiency in the red and infrared parts of

\textsuperscript{1}STAR is an acronym for “natural surface texture and enhanced absorption with back reflector”.

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Figure 4.1: Schematic sketch of a thin-film microcrystalline silicon solar cell (a) on a smooth substrate and (b) on a randomly textured substrate. The periodic unit cell investigated in this chapter is shown in (c). For each unit cell, the period and height of the grating were varied.

the optical spectrum [47, 90]. For the blue and green parts of the optical spectrum, the short circuit current and the quantum efficiency remain almost constant, since the absorption length for blue and green light is significantly smaller than the thickness of the solar cell. Subsequently the blue and green light will be absorbed within the first few hundreds of nanometers of the solar cell. Whilst we observe the enhancements in quantum efficiency by introducing the texturing, in order to fully understand and optimize the nanotexturing process, it is imperative to use numerical models to analyze the optical losses in all layers of the thin-film silicon solar cells [91]. However, the analysis of the wave propagation within a randomly textured solar cell is complex. Therefore as a first learning block, a simple model system based on an integrated grating coupler was selected for investigation. The model system allows for studying the influence of the grating parameters on the solar cell parameters.

A schematic cross section of a microcrystalline silicon solar cell deposited on a smooth substrate and on a randomly textured substrate is shown in Fig. 4.1(a) and 4.1(b), respectively. The microcrystalline solar cell structure, investigated in the study, consists of a 500 nm thick aluminum doped zinc oxide (ZnO:Al) front contact, followed by a hydrogenated microcrystalline silicon p-i-n diode ($\mu$-Si:H) with a total
4.2. Solar Cells on Smooth Substrates

The investigation of solar cells on smooth substrates allows us to gain insights in the optical wave propagation within a microcrystalline silicon solar cell. Furthermore, these simulation results are then used as a reference to compare the performance of cells with integrated grating couplers. The structure of the solar cell on a smooth substrate used in this investigation is consistent with the standard microcrystalline silicon solar cell structure developed by the Research Center Jülich (Institute of Photovoltaics). A detailed description of the device fabrication is given in Ref. [95]. A schematic cross section of a microcrystalline silicon solar cell on a smooth substrate is shown in Fig. 4.2(a). In this simulation based study, the metal back contact of the solar cell was substituted with a perfect reflector. A silver back contact, like those on the fabricated cell, was not used because the optical properties of the zinc-oxide/silver contact is unknown and it also differs significantly if only properties of bulk-silver is used.

The simulations of the optical wave propagation within the solar cell on a smooth substrate were carried out for wavelengths ranging from 300 nm to 1100 nm. The complex refractive indices for each layer were used to simulate the electric field distribution throughout the device structure for the entire wavelength range. Using the electric field distributions, the time average power loss, $Q(x, z)$, within the individual regions of the solar cell was calculated using the equation...
where $c$ is the speed of light in free space, $\epsilon_0$ is the permittivity of free space, $\alpha$ is the energy absorption coefficient $(4\pi k/\lambda)$, with $n$ being the real part of the complex refractive index, and $E(x, z)$ is the electric field. The time average power loss within a microcrystalline silicon solar cell on a smooth substrate is shown in Figs. 4.2(b) and 4.2(c). The incident wavelengths were 400 nm and 700 nm, respectively. It was calculated for an incident wave with an amplitude of 1 V/m. Due to high extinction coefficient of silicon for the shorter wavelengths, the light with 400 nm wavelength is absorbed within the vicinity of zinc-oxide/silicon interface layer. Whereas for the 700 nm wavelength case, the power loss in the silicon layer is dominated by the constructive and destructive interferences of the forward and backward propagating waves. Due to the low absorption coefficient of silicon for longer wavelengths, a large fraction of the light is reflected from the back contact leading to the formation of a standing wave in front of the back contact. In this case, 76% of the incident light is reflected, whereas only 24% of the light is absorbed by the solar cell.

The power loss of a microcrystalline silicon solar cell on a smooth substrate is shown
4.3 Solar Cells with Integrated Gratings Couplers

Different concepts have been proposed to increase the effective optical thickness of silicon solar cells. The suggested concepts range from antireflection coatings,[96, 97] applying optical filters, [98] highly reflective back contacts, [99] utilizing photonic crystals, [100, 101] diffraction gratings, [92, 102–104] to nanotexturing [95] of the contact layers by wet chemical etching. In the case of microcrystalline silicon thin-film solar cells, randomly textured contact layers have been realized by direct growth
of zinc oxide films by low pressure chemical vapor deposition or etching of sputtered zinc oxide [31, 95]. For a superstrate p-i-n microcrystalline silicon solar cell with an i-layer thickness of 1 \( \mu \)m, nanotexturing can lead to an increase in the total short circuit current from 16.3 to 23.4 mA/cm\(^2\) [47]. In our simulation model, we have utilized a simpler line grating model to understand the optical wave propagation within a solar cell. Such grating couplers have been reported in literature as well - different research groups have fabricated amorphous and microcrystalline silicon solar cells where the gratings were created at the glass substrate level [105] or at the front zinc-oxide layer [92, 104]. By having a grating coupler as the textured interface between the zinc-oxide and silicon layer, the absorption within the diode layer would be dominated not only by interference effect, as observed for smooth solar cell cases, but scattering and higher order diffraction will also come onto effect.

In order to compare different grating designs, the quantum efficiency is utilized. The quantum efficiency is defined as the ratio of the power absorbed in the silicon layer with respect to the total power incident, \( P_{opt} \) on the unit cell.

\[
QE = \frac{1}{P_{opt}} \int Q(x, z) dxdz
\]  

The collection efficiency taking the electronic properties of the material into account is assumed to be 100\%. In other words, the internal quantum efficiency is assumed to be 100\%. Therefore, the determined quantum efficiency defines an upper limit of the achievable external quantum efficiency.

4.3.1 Influence of Grating Height on the Absorption in Solar Cells

The simulated power loss profiles for an incident wavelength of 700 nm are shown in Figs. 4.4(b)-4.4(d). The power loss profile was determined for groove heights of 100, 200, and 300 nm, respectively. A comparison of the optical absorption profile in Figs. 4.4(b)–4.4(d) with the absorption profile shown in Fig. 4.2(c), which illustrated the case of a unit cell on a smooth substrate for the same incident wavelength, indicates that the absorption is increased for all groove heights. Scattering and diffraction enhances the effective path length of light inside the silicon absorber layer and as a consequence the absorption for such grooved structure is higher. For small groove heights, the absorption is increased by diffraction effects leading to maxima of the absorption at the boundary of the unit cell. For larger grooves heights Figs. 4.4(c) and 4.4(d), the maxima of the absorption shift toward the center of the unit cell. Catchpole and Green reported that for solar cells with periodic grating couplers, the power loss is maximized, if the phase shift of the grating modes is equal to 180° or its odd multiples [106]. A similar behavior is observed for the case shown in Fig. 4.4(c). The reflections and quantum efficiencies for the different periods are tabulated in Table 4.1.
4.3. Solar Cells with Integrated Gratings Couplers

Figure 4.4: (a) Schematic of a unit cell with a period 700 nm with integrated grating coupler and simulated power loss profile for groove heights (b) 100 nm, (c) 200 nm, and (d) 300 nm under monochromatic illumination (wavelength of 700 nm).

Table 4.1: Reflection and quantum efficiency for different groove heights under monochromatic illumination of wavelength 700 nm. The period of the diffraction grating was kept constant at 700 nm.

<table>
<thead>
<tr>
<th>Groove Height (nm)</th>
<th>Total Reflection (%)</th>
<th>Quantum Efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flat case (0)</td>
<td>76.0</td>
<td>0.20</td>
</tr>
<tr>
<td>100</td>
<td>52.2</td>
<td>0.40</td>
</tr>
<tr>
<td>200</td>
<td>45.1</td>
<td>0.47</td>
</tr>
<tr>
<td>300</td>
<td>65.7</td>
<td>0.27</td>
</tr>
</tbody>
</table>

The zinc oxide/silicon front grating interface works as a phase grating; hence the phase difference can be calculated using the equation

\[ \phi_F = \frac{2\pi}{\lambda} | n_{Si} - n_{ZnO} | h_g \]  

(4.3)

where \( n_{Si} \) and \( n_{ZnO} \) are the real parts of the complex refractive indices of silicon and zinc oxide, respectively, with \( h_g \) being the groove height of the line grating. For a grating structure with a groove height of 200 nm, the phase difference is almost 180° which results into the highest quantum efficiency for the values shown in Table 4.1. As the phase shift drifts away from this value with increasing groove height, a drop in the quantum efficiency is observed. Furthermore, with increasing groove height, the front...
4. µc-Si Solar Cells with Integrated Lamellar Gratings

Figure 4.5: Diffraction orders for structures with grating heights of (a) 180 nm and (b) 360 nm.

zinc oxide layer starts absorbing more of the longer wavelength, so that the absorption of the silicon diode is reduced as well.

To gain insights in the optics of textured solar cells, the influence of the front and the back grating on the wave propagation was investigated separately. We will start with the front grating. By varying the grating height the phase difference (calculated from Eq. 4.3) of the interfering waves is changed. For simplicity we will concentrate in the following on two cases: a phase change of $\pi$ and $2\pi$. In the case of farfield diffraction (Fraunhofer diffraction), a phase difference of $\pi$ results in the propagation of even diffraction orders [69]. As a result, the zero order is canceled out and light is diffracted and transmitted only at orders $m = \pm 1, \pm 3, \ldots \pm 2n + 1$ etc. as shown in the sketch in Fig. 4.5(a). Hence, all light propagates at large diffraction angles, which increases the optical path length of the light in the solar cell. For a grating structure causing a phase change of $\pi$ and an incident wavelength of 700 nm the corresponding grating height of the front grating was calculated to be 180 nm.

Similarly, for a grating structure with a phase difference of $2\pi$ destructive interference of the odd diffraction orders is observed, so that only even diffraction orders can propagate ($m = 0, \pm 2, \pm 4, \ldots \pm 2n$ etc.) as shown in Fig. 4.5(b). Hence, a large fraction of the transmitted light propagates in the 0th order. In this case the optical path length of the light is reduced in comparison to the grating generating a phase difference of $\pi$. For a phase difference of $2\pi$ and an incident wavelength of 700 nm the corresponding grating height of the front grating was calculated to be 360 nm.

We will continue with the back grating. The back grating acts as a reflection grating. It diffracts and reflects the incident light transmitted through the front grating. The phase difference introduced by the back grating can be calculated by:
4.3. Solar Cells with Integrated Gratings Couplers

4.3.1. Specular and Diffused Transmission

Figure 4.6: (a) Specular and (b) diffused transmission for zinc-oxide/silicon front gratings on an infinite silicon substrate. The period of the front grating was 700 nm.

\[ \phi_B = \frac{4\pi}{\lambda} \cdot n_{Si} \cdot h_g \] (4.4)

where \( n_{Si} \) is the real part of the complex refractive index of silicon with \( h_g \) being the groove height of the line grating. The phase difference of the back grating can be controlled by the grating height. The influence of the front and the back grating on the wave propagation was studied by calculating the diffraction pattern of the front and the back grating separately. To analyze the diffraction behavior of the solar cells as a function of the wavelength we used the Rigorous Coupled Wave Analysis [78, 85]. By using the Rigorous Coupled Wave Analysis we can calculate the diffraction efficiency of the transmitted and reflected waves for the different orders as a function of the incident wavelength.

In Figs. 4.6(a) and 4.6(b), contour plots of the specular and diffused transmission of the front grating for a grating period of 700 nm is shown. The transmission was calculated for a front grating fabricated on top of an infinite silicon slab to study the behavior of the front grating. The diffused transmission is defined as the transmitted light that is diffracted in diffraction orders other than the 0th order. If the phase change introduced by the front grating is equal to \( \pi \), the light is diffracted in the odd orders \( m = \pm 1, \pm 3, \ldots \pm 2n + 1 \). Consequently, most of the light contributes to the diffused transmission, while the specular transmission is minimal. The red line with
Figure 4.7: (a) Specular and (b) diffused reflection for silicon/metal back gratings on an infinite silicon substrate. The period of the back grating was 700 nm.

Similar to the transmission of the front grating of the solar cell, the specular and diffused reflection were calculated for the back grating. The simulated reflection for a grating period of 700 nm is shown in Figs. 4.7(a) and 4.7(b). The specular reflectance is shown in Fig. 4.7(a). For a grating height corresponding to $\pi$, the specular
4.3. Solar Cells with Integrated Gratings Couplers

Figure 4.8: Comparison of quantum efficiency for cell on smooth substrate with grating couplers with a groove height of 300 nm and periods of 600 and 3000 nm.

reflectance has a minimal value. For such a structure, when the light reaches the back grating it is diffracted in the higher orders and almost no light is reflected straight into the zero mode. The specular reflectance is maximized, when the back grating creates a phase difference of $2\pi$ and its even multiples. Fig. 4.7(b) presents a contour map of the diffuse reflection of the back grating. The diffuse reflectance is maximized for a phase difference of $\pi$ or odd multiples of $\pi$. As for the case of $2\pi$ and its even multiples, the diffuse reflectance is minimal, since a large portion of the light is reflected into the zero order. The observations in Figs. 4.7(a) and 4.7(b) comply with the derivations and theoretical explanation in Eq. 4.4. For a wavelength of 700 nm, phase difference of $\pi$ is generated by a back grating of 46 nm or its odd multiples, while for a phase difference of $2\pi$ a back grating with a height of 92 nm or its even multiples is required. The RCWA analysis confirms that a small variation of the grating height has a more influential effect on the back grating than on the front grating.

4.3.2 Influence of Grating Dimensions on the Short Circuit Current

The influence of the grating structure on the absorption profile for different wavelengths were studied for the solar cell structures simulated using the FDTD method. The simulated quantum efficiency as a function of the wavelength is shown in Fig. 4.8. The quantum efficiency was simulated for a solar cell on a smooth substrate [Fig.
4.2(a)] and grating structures [Fig. 4.4(a)] with different periods of 600 and 3000 nm. The groove height was chosen to be 300 nm for the grating structures. Introduction of a grating leads to an increase in the quantum efficiency for a period of 600 nm. The quantum efficiency is distinctly increased in the red and the infrared part of the optical spectrum, whereas the grating coupler has almost no influence on the quantum efficiency for shorter wavelengths. Furthermore, the influence of the period on the quantum efficiency is illustrated in Fig. 4.8. For a small period of 600 nm, a distinct increase in the quantum efficiency is observed, whereas for the larger period of 3000 nm, the quantum efficiency almost converges against the quantum efficiency of the solar cell on a smooth substrate. A summary of the simulated quantum efficiencies and the reflection of the solar cells for a wavelength of 700 nm and a grating period of 700 nm are given in Table 4.1. The highest quantum efficiency was achieved for a groove height of 200 nm.

In order to compare the different grating designs, the short circuit current was calculated for red and infrared illuminations 600–1100 nm. To obtain the short circuit current, $I_{SC}$, the product of the wavelength dependent AM 1.5 spectral irradiance, $S$, and the spectral response, $SR$, was integrated over the red and infrared parts of the optical spectrum. The short circuit current can be calculated by

$$I_{SC} = \int SR(\lambda)S(\lambda)d\lambda, \quad \text{with} \quad SR(\lambda) = \frac{q\lambda}{hc}QE(\lambda)$$

where $q$ is the elementary charge, $\lambda$ is the wavelength, $h$ is the Planck constant, and $c$ is the speed of light. The short circuit current as a function of the groove height is shown in Fig. 4.9 for different periods of the unit cell.

The dashed line exhibits the short circuit current for a solar cell on a smooth substrate [Fig. 4.2(a)]. A short circuit current of 5.6 mA/cm$^2$ was calculated for such structure. Compared to the value calculated for the flat case, introduction of a groove leads to a higher short circuit current irrespective of the period size and the groove height. The highest short circuit current is observed for a period of 600 nm and a groove height of 300 nm. In comparison to the smooth substrate, the short circuit current is increased by a factor of 2.1 resulting in a short circuit current of 11.3 mA/cm$^2$. The enhancement or gain factor, $G$, can be expressed by

$$G = \frac{\int SR_g(\lambda)S(\lambda)d\lambda}{\int SR_s(\lambda)S(\lambda)d\lambda}$$

where $SR_s$ is the spectral response of a solar cell on a smooth substrate and $SR_g$ is the spectral response of a solar cell with integrated diffraction grating. A comparison of the curves for grating periods of 500, 600, and 700 nm indicates that the highest short circuit current is observed for groove heights of 200, 300, and 400 nm. Therefore, the
4.3. Solar Cells with Integrated Gratings Couplers

Figure 4.9: Short circuit current for different grating parameters under red illumination (wavelength of 600–1100 nm) as a function of groove height of the unit cell.

Short circuit is maximized if the groove height is approximately equal to half of the grating period.

The short circuit current as a function of the period for different groove heights is shown in Fig. 4.10. With increasing period, a drop of the short circuit current can be observed for all groove heights. The observation can be explained by using the grating equation [73]

\[ P \cdot n \cdot \sin(\theta_m) = m\lambda \]  

where \( P \) is the period of the grating, \( n \) denotes the refractive index of the propagating media after diffraction, \( m \) specifies the diffraction order, and \( \theta_m \) being the diffraction angle. As the period is increased, the diffraction angle for an integrated grating coupler is reduced. Consequently, the effective thickness of the solar cell is reduced. With increasing period size, the effective thickness will converge toward the real thickness of the solar cell, which implies that the optical path length of the cell is reduced for larger periods compared to shorter periods of the unit cell. Subsequently, the short circuit current converges against the short circuit current of a microcrystalline silicon thin-film solar cell on a smooth substrate.
4. **μc-Si Solar Cells with Integrated Lamellar Gratings**

![Graph showing short circuit current vs. period for different groove heights and wavelengths.](image)

**Figure 4.10:** Short circuit current for different grating parameters under red illumination (wavelength of 600–1100 nm) as a function of period of the unit cell.

### 4.3.3 Comparison of Optical Simulations and Experimental Results

Microcrystalline silicon solar cells with integrated grating structures exhibit an enhanced short circuit current. For short wavelengths, the line grating has only a small influence on the short circuit current, whereas a distinct increase in the photocurrent is observed for longer wavelengths. In the following, the simulations will be compared to experimental results in literature. Senoussaoui et al. [92] realized microcrystalline silicon solar cells with integrated grating couplers. The design of the solar cell with integrated grating couplers was identical with structures investigated in this study. Solar cells on smooth substrates exhibit short circuit currents of 5.8–6.6 mA/cm² measured under red illumination applying an optical filter, OG 590, wavelength range 600–1100 nm. For solar cells with integrated grating couplers, the short circuit current under red illumination ranged from 7.3 to 9.5 mA/cm². The grating period was varied from 1.2 to 4.0 µm. Structures with smaller grating periods were not realized in this study. The highest short circuit current of 9.5 mA/cm² was observed for a grating period of 1.5–2.0 µm and a groove height of 400 nm. Solar cells on randomly textured surfaces exhibit short circuit currents of 10.0–11.0 mA/cm². The numerical simulations in this study exhibit a short circuit current wavelength 600–1100 nm for smooth substrates of 5.6 mA/cm², and a short circuit current of 8.95 mA/cm² for a period of 1200 nm and a groove height of 400 nm. Therefore, the experimental results and the simulations...
Table 4.2: Comparison of experimental results with numerically simulated short circuit current under red illumination wavelength range 600–1100 nm for solar cells with grating couplers of groove height 400 nm and three different grating periods. (N.B. While period 1.6 µm was fabricated in Ref. [92], this study investigated a period of 1.5 µm).

<table>
<thead>
<tr>
<th></th>
<th>Experimental results</th>
<th>Numerical Simulations</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Absolute value (mA/cm²)</td>
<td>Relative increase (%)</td>
</tr>
<tr>
<td>Smooth Substrate</td>
<td>5.8-6.6</td>
<td>5.6</td>
</tr>
<tr>
<td>Period: 1.2 µm</td>
<td>8.5</td>
<td>29.3</td>
</tr>
<tr>
<td>Period: 1.6/1.5 µm</td>
<td>9.5</td>
<td>46.1</td>
</tr>
<tr>
<td>Period: 3.0 µm</td>
<td>8.55</td>
<td>30.7</td>
</tr>
</tbody>
</table>

exhibit a good agreement.

The numerical simulations exhibit a maximum of the short circuit current under red illumination for a grating period of 600 nm and a groove height of 300 nm. A comparison of the experimental results by Senoussaoui et al. [92] and the simulation results in this study for different periods is given in Table 4.2. It has to be noted that the collection efficiency was assumed to be 100% in the simulations leading to an internal quantum efficiency of 100%.

A comparison of the experimental results presented by Senoussaoui et al. for periodic grating structure and randomly textured substrates exhibits distinctly higher short circuit currents for randomly textured solar cells. Therefore, the simulations results in this chapter present the first step in investigating more complex structures such as periodically arranged pillar gratings, pyramids, or quasi-random arrangements of pillars/pyramids, which cannot be fully understood by simple analytical models.

### 4.4 Toward an Optimal Grating Structure

In order to maximize the short circuit current and the quantum efficiency, the diffraction of the integrated grating should be high. Different solar cell structures with integrated grating designs have been proposed in literature. Haase et al. [108] investigated a microcrystalline silicon thin-film solar cell with an integrated line grating by a using a finite integration method approach. The investigated device structure is identical with the structures characterized in this study. They reported that the short current is maximized if the grating period is equal to 700 nm and the groove height is equal to 330 nm. The width of the groove of the diffraction grating was assumed to be 50%.
In their investigation, they tried to maximize the short circuit current for a wavelength range from 700 to 1100 nm. A comparison with the result presented in this chapter shows that the dimensions at which the short circuit current is maximized are very similar.

An optimal period and groove height can also be determined by simple analytical modeling of diffraction gratings using a modal method [106, 109]. Catchpole and Green applied the modal method to analyze the incoupling of light into a solar cell. They derived an optimal grating period of 650 nm and a groove height of 300 nm for a ZnO/silicon grating structure [106]. The reported design of the grating parameters is very close to the parameters determined in this study. Therefore, the method presented by Catchpole and Green provides a rather simple approach to determine the optimal grating parameters.

In terms of the short circuit current and the quantum efficiency, it is difficult to compare the different methods. The method proposed by Catchpole allows for the analysis of front gratings. The method does not allow for the analysis of the double grating discussed in this study. Therefore, the numerical simulation of the power loss in the device is necessary to determine an upper limit of the short circuit current and the quantum efficiency. Furthermore, the influence of the manufacturing process on the actual layer sequence of the solar cell has to be taken into account when modeling the light propagation in such a structure. And this is only possible by using a model that numerically calculates the power loss profile for the given structure. In the current manuscript, a microcrystalline silicon solar cell in superstrate configuration was investigated. The texturing was introduced by patterning the doped zinc oxide window layers. In order to investigate the influence of the front or back grating on the short circuit current and quantum efficiency, the layer sequence has to be adjusted. A microcrystalline silicon solar cell with a textured front contact and a smooth back contact can only be realized by using a solar cell in substrate configuration.

A comparison of different device structures reveals that the solar cell with a double grating is clearly superior to a structure with a front or a rear grating only. In Fig. 4.11 the short circuit current is shown for solar cells with only one, either front or back, grating. When studying solar cells with separate line gratings in the front and back, the fabrication process of the cells has to be taken into account. A solar cell with a front grating but no back grating can only be realized by fabricating a solar cell in substrate configuration, as it is shown in the inset of Fig. 4.11(a). A solar cell with a textured back contact, as shown in the inset of Fig. 4.11(b), can be realized by fabricating a solar cell in superstrate configuration. The back contact of the solar cell has to be textured, while the front contact remains untextured. In the case of a solar cell with a front grating, the short circuit current increases under red illumination 600–1100 nm by 2.0–4.0 mA/cm², whereas for a solar cell with a back grating, the
4.4. Toward an Optimal Grating Structure

Figure 4.11: Short circuit current under red illumination (wavelength 600-1100 nm) of a microcrystalline silicon thin-film solar cell with only an integrated (a) front or (b) back grating as a function of grating period for different grating heights.

The short circuit current increases by 2.0–2.5 mA/cm$^2$. The double grating structure leads to an increase in the red and the infrared current by 7.0 mA/cm$^2$. Therefore, the interaction between the front and the rear grating plays a significant role in increasing the short circuit current. A systematic study of such structures is essential to improve the understanding of the wave propagation in microcrystalline silicon solar cells and improve the overall conversion efficiency.

Tuning the Phase Gratings

The optical simulations of solar cells with integrated line grating indicate that the short circuit current is maximized for a grating height of $2\pi$. In this case the front grating transmits a large fraction of the incident light, which is reflected and effectively diffracted by the back grating at larger diffraction angles. The efficiency of the solar cell is maximized if the incident light is efficiently coupled in and transmitted straight into the structure by the front grating and then strongly diffracted by the back grating. The light is transmitted straight into the structure, when the front grating causes a phase difference of $2\pi$. The back grating has to correspond to a phase difference of $\pi$ in order to strongly diffract the incoming light into the higher diffraction orders. The quantum efficiency of the solar cell with a grating height of 180 nm, 340 nm and 360nm for an incident light spectrum from 300 nm to 1100 nm is shown in Fig. 4.12. Of these three structures, the highest short circuit current was achieved for a grating height of 340 nm. The three structures exhibit similar quantum efficiency for shorter wavelengths ($< 550$ nm). Short wavelengths are absorbed within the first
few nanometers of the solar cell due to the strong wavelength dependent absorption coefficient of microcrystalline silicon. Only a fraction of the light reaches the back contact, where it is diffracted. Beyond wavelength of 550 nm the absorption profile of the solar cell is determined by interference and superposition of the diffraction modes of the front and the back grating. The structures with a grating height of 360 nm and 340 nm exhibit higher quantum efficiencies than the structure with a grating height of 180 nm for the wavelengths from 650 nm to 750 nm. For a grating height of 180 nm the corresponding phase differences of the front grating is equal to π and the back grating causes a phase shift of 1.7π. As a consequence a large fraction of the incident light reaches the back contact where it is diffracted in the 0th order resulting in an increased reflection of the solar cell. Subsequently the quantum efficiency is low for this wavelength region. A grating height of 360 nm results in a phase difference of 2π for the front grating and 1.4π for the back grating. The phase difference of the front grating matches the optimization rule, however the phase difference for the back grating is still relatively far away from the optimal phase change of π. A grating with a height of 340 nm causes a phase change of 1.9π (approximately 2π) in the front and the phase change of π in the back. As a result, the solar cell with 340 nm grating height exhibits the highest QE. The optimized structure exhibits an advantage of the QE in the region 625 nm – 750 nm, since the structure was adjusted for optimal performance for wavelength of 700 nm. As a next step the short circuit current was calculated for the

Figure 4.12: Quantum efficiency of solar cells structures with period 700 nm and grating heights of 180 nm, 340 nm and 360 nm.
### Table 4.3: Phase difference and short circuit current data for solar cells with period 700 nm and heights of 180 nm, 340 nm and 360 nm.

<table>
<thead>
<tr>
<th>Grating Height [nm]</th>
<th>Phase Difference [radian]</th>
<th>Short Circuit Current [mA/cm²]</th>
</tr>
</thead>
<tbody>
<tr>
<td>180 nm</td>
<td>Front: $\pi$</td>
<td>16.3</td>
</tr>
<tr>
<td></td>
<td>Back: $1.7\pi$</td>
<td></td>
</tr>
<tr>
<td>340 nm</td>
<td>Front: $1.9\pi$</td>
<td>19.1</td>
</tr>
<tr>
<td></td>
<td>Back: $\pi$</td>
<td></td>
</tr>
<tr>
<td>360 nm</td>
<td>Front: $2\pi$</td>
<td>18.5</td>
</tr>
<tr>
<td></td>
<td>Back: $1.4\pi$</td>
<td></td>
</tr>
</tbody>
</table>

three structures. The short circuit current values are summarized in Table 4.3. The short circuit current of the solar cell with a grating height of 340 nm and 360 nm is significantly higher (2.2-2.8 mA/cm²) than the current of a structure with a grating height of 180 nm. The solar cell with a grating height of 360 nm exhibits a short circuit current of 18.5 mA/cm², which is 2.2 mA/cm² higher than the structure with 180 nm grating height (16.3 mA/cm²). The optimal grating structure with a grating height of 340 nm leads to another increase of the short circuit current by 0.6 mA/cm², resulting in a short circuit current of 19.1 mA/cm².

The derived design rules are not limited to microcrystalline silicon thin-film solar cells. The concept can be easily transferred to other thin film solar cells with integrated line grating. We have tested the design rules for amorphous silicon thin film solar cells. For an amorphous silicon solar cell with a thickness of 350 nm, we found optimal grating periods of 300 nm and optimal grating heights of 200 nm. Due to the large optical bandgap of 1.75 eV longer wavelength cannot be efficiently absorbed by the solar cell. Therefore, the optimal short circuit current is observed for smaller grating periods. Smaller grating periods allow for the efficient scattering of short wavelengths, which can be efficiently absorbed by the solar cell. The highest short circuit current is again observed for a front grating phase difference of close to $2\pi$ and a back grating phase shift of close to $\pi$.

A topic for further investigation is the separate control of the front and the back grating height in an attempt to achieve the optimal phase change. For example the adjustment of the thickness of the zinc oxide layer between the microcrystalline diode and the back contact allows for tuning the phase change of the back contact. As an alternative different materials can be used to form a back contact in the solar cell structure.

In terms of designing a microcrystalline solar cell with integrated diffraction grating, the following design rules can be derived: The period of the diffraction grating
should be small, so that the light is diffracted at large diffraction angles. However, if the period is too small, higher order diffraction modes cannot propagate in the solar cell structure anymore. The constructive interference of modes in the device structure plays an essential role in optimizing the solar cell design. A detailed modal analysis of solar cells with nanotextured surfaces was developed by Catchpole [109]. If the grating period is too small, only zeroth and first order diffraction modes can propagate in the thin-film solar cell. Subsequently the short circuit current is distinctly reduced, since high order diffraction modes cannot propagate anymore. In the case of a microcrystalline silicon solar cell with an integrated diffraction grating, such behavior is observed for grating periods smaller than or equal to 450 nm. The maximum of the short circuit current is observed if a grating period is equal to 600 nm. After determining the optimal period of the diffraction grating, the groove height has to be determined. The numerical simulations show that for a given period, the short circuit current is maximized if the groove height is approximately equal to half of the grating period. The investigated microcrystalline silicon solar cell exhibits a maximum of the short circuit for a groove height of 300 nm.

4.5 Summary

In this chapter the wave propagation in microcrystalline silicon thin-film solar cells with integrated grating couplers was investigated using a Finite Difference Time Domain and Rigorous Coupled Wave Analysis approach. The influence of the grating period and the grating height on the short circuit current and the quantum efficiency was investigated. The quantum efficiency in the blue part of the optical spectrum is almost unchanged, whereas a distinct increase in the quantum efficiency was achieved in the red and the infrared part of the spectrum. The period of the diffraction grating should be small, so that the light is diffracted at larger diffraction angles. However, if the grating period is too small, high order diffraction modes cannot propagate and subsequently the short circuit current drops. Furthermore the interaction of the front and the back grating plays a major role in optimizing the short circuit current of the solar cells. The short circuit is maximized if the phase change of the front grating is close to $2\pi$, whereas the phase change of the back grating is close to $\pi$. In comparison to a microcrystalline solar cell on a smooth substrate, the red and infrared currents are increased by more than 100%. The total short circuit current (wavelength 300–1100 nm) is increased by 7.04 mA/cm² that sums up to 19.7 mA/cm². The numerical simulations were compared with experimental results in literature and a good agreement was observed. In terms of design rules for microcrystalline silicon solar cells with integrated diffraction grating, it was found that the short circuit current can be maximized if the groove height is approximately equal to half of the grating period.
Chapter 5

\(\mu c\)-Si Solar Cells with Triangular Texture

In this chapter, the surface texture in thin-film silicon solar cells were approximated with triangular texture. These periodic triangular gratings were integrated in solar cells and the influence of the profile dimensions on the quantum efficiency and the short circuit current was studied. By identifying the influence of the period and height of the triangular profile, the design of the structures were optimized to achieve higher short circuit currents and quantum efficiencies. Compared to the study with lamellar gratings in the previous chapter, a wider range of periods of the unit cell were swept in this study. Enhancement of the short circuit current in the blue part of the spectrum is achieved for small triangular periods (\(P<200\) nm), whereas the short circuit current in the red and infrared part of the spectrum is increased for triangular periods (\(P = 900\)nm) comparable to the optical wavelength.

5.1 Optical Simulation Model

With an absorber layer in the range of 1 \(\mu\)m, complete utilization of light incoupling and light trapping is imperative for realizing efficient thin-film solar cells based on microcrystalline silicon (\(\mu c\)-Si:H) or amorphous silicon (a-Si:H) [56, 110]. Efficiencies higher than 10% have been achieved for microcrystalline silicon solar cells by introducing textured interfaces in the solar cell [6, 23, 95, 111]. By considering the near field optics, the nano texturing process for efficient solar cells can be understood and optimized. To model the nanotexturing, in the previous chapter, a simple model system based on an integrated grating coupler was selected. In this study the nano texturing of the front interface of the microcrystalline solar cell property was investigated by introducing a triangular grating which represents the textured front interface of a real thin-film silicon solar cell. Triangular and pyramidal structures have been extensively
investigated for solar cell applications in the past decade [97, 112, 113]. But they were mostly addressed for crystalline silicon solar cells, where the period of the structures were larger than the wavelength of the incident light in many folds. Hence, geometric optics was sufficient to understand the behavior of optics for such solar cells. A recent paper has studied pyramidal textures in thin-film silicon solar cells [11]. However, the manuscript does not provide a detailed description of the wave propagation for small surface textures. Such small textures have distinct influence on the incoupling of blue light in the solar cell.

As mentioned in previous chapters, two of the widely used approach to form a textured layer are: by direct growth of zinc oxide films by low pressure chemical vapor deposition or etching of sputtered zinc oxide [31, 95]. A surface profile of such an etched aluminum doped zinc oxide (ZnO:Al) is shown in Fig. 5.1(a). The sputtered zinc oxide film was etched for 10 seconds in a 0.5% diluted hydrochloric acid (HCl) solution. Fig. 5.1(a) shows a three dimensional surface profile of the substrate. Surface texturing of the film leads to surface morphology that very closely resembles a pyramid-like structure, albeit not perfectly symmetrical ones.

A line profile of the nanotextured surface is shown in Fig. 5.1(b). In this figure, the triangular profiles exhibit an almost periodic arrangement with a period of around 500 nm. Based on these observations, the model investigated in this study consisted of periodic arrangements of triangular gratings. A schematic cross section of the investigated unit cells is shown in Fig. 5.1(c). The microcrystalline silicon solar cell structure con-
sists of a 500 nm thick aluminum doped zinc oxide (ZnO:Al) front contact, followed by a (p-i-n) hydrogenated microcrystalline silicon diode (µc-Si:H) with a total thickness of 1000 nm and a back reflector consisting of an 80 nm thick ZnO:Al layer and a metal reflector. The device structure is consistent with the standard microcrystalline silicon solar cell process used by several research groups like the Research Center Jülich and University of Neuchâtel [92, 93]. In this study the period of the unit cell and height of the triangular profile was varied. The period of the unit cell was varied from 50 nm up to 6000 nm and the height was varied from 0 nm up to 500 nm. Alternatively, the triangular structure can be described by the opening angle of the triangle, which was varied from $6^\circ$ to $176^\circ$. The unit cell was illuminated under normal incidence for the entire spectrum of wavelength 300 – 1100 nm. The complex optical constants used in the model system were determined by optical measurements of the individual layers. Since a two dimensional FDTD algorithm was utilized, it splits the Maxwell’s equations into two independent sets of equations for transverse electric (TE) and transverse magnetic (TM) polarized waves. The polarization of the input wave was assumed to be TE, thus only one component of the electric field, $E_y$, had to be solved.

## 5.2 Simulation Results

### 5.2.1 Influence of Opening Angle on the Absorption in Solar Cells

In order to compare different textured designs the power loss profiles within the solar cell, the quantum efficiency, the short circuit current were utilized. Since we are still dealing with a 2 dimensional problem, the power loss can be calculated using Eq. 4.1 on page 46 from the previous chapter. The power loss profile for thin film solar cells with integrated triangular textures under blue and red illumination are shown in Fig. 5.2.

The period of the triangular profile for all the cases was 900 nm with heights of 100 nm [Figs. 5.2(a) and 5.2(c)] and 400 nm [Figs. 5.2(b) and 5.2(d)], respectively. The incident light has a wavelength of 400 nm and 700 nm with amplitude of 1 V/m. In the case of short wavelength illumination ($\lambda = 400$ nm) photons get absorbed within the first 200 nm of the silicon absorber layer. The high absorption coefficient of silicon for wavelength 400 nm inhibits the propagating wave to hit the back reflector. By having a small period height, like in Fig. 5.2(a), the opening angle is close to $180^\circ$. Hence the high power loss pattern concentrated around the front interface almost resembles that of a solar cell on a smooth substrate; it is almost continuous along the boundary. Whereas, by having an opening angle close to $90^\circ$, a “flamelike” power loss pattern is seen in Fig. 5.2(b). The “flame-like” power loss pattern is caused by the formation of evanescent fields at the boundary between the zinc oxide texture and the
pin solar cell. Such “flame-like” patterns are observed because the refractive index difference between zinc oxide and silicon is relatively large for short wavelengths. As a consequence a relative large fraction of the incident light is reflected by the interface. Due to the triangular shape of the interface, a standing wave pattern is formed in the region close to the tip of the triangle. Since the electric field at the boundary between zinc oxide and the silicon diode cannot be discontinuous, an evanescent field extends in the silicon diode. The “flame-like” power loss pattern disappears for longer wavelength and smaller periods of the texture.

Due to a low absorption coefficient of silicon for longer wavelengths, the incident light has to be confined in the solar cell. Only if the light completes multiple passes inside the silicon layer the light can be completely absorbed. The power loss profile for a structure under monochromatic illumination of wavelength 700 nm is shown in Figs. 5.2(c) and 5.2(d). Diffraction from the front and back grating constructively interfere towards higher absorption. Within the multiple passes, the diffracted light interferes with the backward propagating waves and also with other diffracted waves from neighboring unit cells. By following the path of the different diffracted orders from the front and back grating, the highest intensities are observed where the second diffraction (front grating) orders from the neighboring cells meet at the center of the unit cell. A similar behavior is observed for lamellar gratings integrated in microcrystalline silicon solar cells [114]. The diffraction from the back reflection does not play
a significant role in creating high intensities at the center of the unit cell. But the back grating contributes to the formation of high power losses close to the back reflector. The power loss close to the back reflector depends on the confinement angle of the back reflector. If the opening angle is close to $90^\circ$, the power loss close to the back reflector, as seen in Fig. 5.2(d), is maximized.

### 5.2.2 Influence of Profile Dimensions on the Short Circuit Current

In the next step the quantum efficiency was determined. The quantum efficiency is defined as the ratio of the power absorbed in the silicon layer with respect to the total power incident on the unit cell. Details on how to calculate the quantum efficiency were given in the previous chapter. It can be calculated using Eq. 4.2 on page 48. The collection efficiency taking the electronic properties of the material into account is assumed to be 100%. In other words, the internal quantum efficiency is assumed to be 100%. Therefore, the determined quantum efficiency defines an upper limit of the achievable external quantum efficiency. The calculated quantum efficiency is shown in Fig. 5.3 for a solar cell on a flat substrate, and two solar cells with integrated triangular gratings. The triangular profiles have periods of 100 nm and 900 nm, both with a profile height of 400 nm. For shorter wavelengths (300 – 500 nm), the quantum efficiency for the solar cell with a texture period of 100 nm is higher than that of the flat case. But with increasing wavelength, both devices exhibit the same quantum efficiency. The thickness of the p-layer of the microcrystalline silicon p-i-n solar cell was assumed to be 30 nm for all the cells. For small and very small texture periods ($P \leq 200$ nm) the grating acts as effective index matching layer, so that the incoupling of light with short wavelength is improved. Due to the enhanced incoupling, the quantum efficiency for the shorter wavelengths is increased, whereas it remains almost unchanged for longer wavelengths (600 - 1100 nm). For longer wavelengths, the solar cells with grating period of 900 nm exhibit distinctly enhanced quantum efficiency compared to a solar cell on smooth substrates. Compared to that of a solar cell on smooth substrates, the optical path length is increased. For the blue and green part of the optical spectrum the quantum efficiency remains almost constant, since the absorption length for blue and green light is significantly smaller than the thickness of the solar cell. Subsequently the blue and green light will be absorbed within the first few hundred nanometers of the cell.

Based on the quantum efficiency, the short circuit current was calculated for the standard AM 1.5 weighted sun spectra using Eq. 4.5 on page 54. The influence of the grating dimensions on the short circuit current in blue and the red/infrared part of the optical spectrum is shown in Figs. 5.4(a) and 5.4(b) as a function of the grating period. In Fig. 5.4(a) the short circuit current was calculated for a spectral range from
Figure 5.3: Comparison of quantum efficiency for solar cell on smooth substrate with triangular structures of height 400 nm and periods of 100 nm and 900 nm.

$\lambda_{\text{min}} = 300$ nm to $\lambda_{\text{max}} = 500$ nm. The dashed line represents the short circuit current of a solar cell on a flat substrate. For larger texture periods the short circuit current is comparable to the solar cell on flat substrates. Due to the small penetration depth in this range of the spectrum, light trapping is negligible. For smaller and very small periods an enhancement of the short circuit current is observed. The enhancement of the short circuit current is caused by an improved incoupling of the light. Compared to that of a solar cell on a smooth substrate, enhanced short circuit current in this spectral range is increased from 2.9 mA/cm$^2$ to 3.6 mA/cm$^2$. This increase in the short circuit current is observed for periods smaller than 200 nm. For such small periods the wavelengths of the incident light is much larger than the period of the triangular grating, so that the triangular grating acts as an effective refractive index gradient. The refractive index linearly increases from a refractive index of zinc oxide to the index of microcrystalline silicon. As a consequence the reflection at this particular interface is reduced and more light is coupled in the solar cell. If the grating period is smaller than $\lambda/2n$, where $\lambda$ is the wavelength of the incident light and $n$ the refractive index of the grating, the behavior of the grating can be described by an effective refractive index gradient. The effective refractive index, $n_{\text{eff}}$, at the front zinc oxide/silicon interface can be calculated based on

$$n_{\text{eff}}(h) = n_{\text{ZnO}} \times \frac{W_{\text{Tex}}(h)}{P_{\text{Unit}}} + n_{\text{Si}} \times \frac{P_{\text{Unit}} - W_{\text{Tex}}(h)}{P_{\text{Unit}}} \quad (5.1)$$
5.2. Simulation Results

Figure 5.4: Short circuit current for different triangular profile heights as a function of the period of the unit cell under (a) blue illumination (wavelength 300 – 500 nm) and (b) red and infrared illumination (wavelength 700 – 1100 nm).

where $W_{T_{ex}}$ is the width of the surface texture as a function of the texture height. $P_{Unit}$ is the period of the unit cell. $n_{ZnO}$ and $n_{Si}$ are the refractive indices of zinc oxide and silicon, respectively, which are the first and second medium as the incident light passes through inside the solar cell. In case of the triangular grating from this study, the effective refractive index is given by

$$n_{eff}(h) = n_{ZnO} + \frac{h}{H_g}(n_{Si} - n_{ZnO})$$

where $h$ is the height of the surface texture and $H_g$ is the maximum height of the surface texture. Due to the symmetry in a triangular grating, the value of $n_{eff}$ increases linearly as it changes from the value of $n_{ZnO}$ to subsequently $n_{Si}$. The triangular grating can be approximated by an effective refractive index gradient for periods equal to or less than 100 nm. For texture periods larger than 200 nm the short circuit current starts converging towards the value calculated for the solar cell on a smooth substrate.

The short circuit current under red and infrared illumination (from $\lambda_{min} = 700$ nm to $\lambda_{max} = 1100$ nm) as a function of the period is shown in Fig. 5.4(b). The highest short circuit current is achieved for periods of 700 nm and 900 nm and a triangular profile height of 400 nm to 500 nm. Compared to the short circuit current of a solar cell on a smooth substrate, the short circuit current is increased by almost 200% from 2.5
mA/cm² to 7 mA/cm². The gain in the short circuit current for this part of the optical spectrum is due to light trapping of the incident light inside the silicon absorber layer. Figure 5.4(b) can be divided into three regions. For texture periods much smaller than the incident wavelength, the triangular grating can be described by an effective refractive index gradient. One might expect an effect similar to the previously described situation under blue illumination. However, the refractive index difference between zinc oxide and microcrystalline silicon is small for longer wavelengths, whereas the refractive index difference for short wavelength is relatively large. In order to illustrate this difference in the refractive indices, the linear change of the refractive index as function of the height is shown in Fig. 5.5. The cases for wavelengths 400 nm and 800 nm are depicted in the figure. In terms of the refractive index value change, the incident light travels through from \( n_{\text{ZnO}-400} = 2.02 \) to \( n_{\text{Si}-400} = 5.56 \) for the shorter wavelength and from \( n_{\text{ZnO}-800} = 1.79 \) to \( n_{\text{Si}-800} = 3.69 \) for the longer wavelength. For a wavelength of 400 nm, 21% of the incoming light is reflected by the interface between zinc oxide and microcrystalline silicon, whereas the reflection is reduced to 12% for a wavelength of 800 nm. Therefore, the effective refractive index gradient has a distinct influence under blue illumination, whereas the influence is significantly reduced for red and infrared illumination.

For texture periods which are much larger than the incident wavelengths (Period > 3 \( \mu \text{m} \)); the short circuit current drops as well. With an increasing period, the diffraction angle for the integrated triangular grating is reduced. Henceforth the diffracted orders
5.3 Parasitic Absorption Losses

Do not interfere with diffracted orders from neighboring unit cells. The constructive interference of the diffracted orders is essential for effectively trapping light inside the absorber layer. Thus the short circuit current for such large texture periods converges towards that of a solar cell on a flat substrate.

If the period of the triangular grating is comparable to the incident wavelengths the diffraction angles are large enough to propagate into their neighboring unit cell. Diffracted waves can thus interfere constructively within the thin absorber layer contributing to the higher short circuit current that is observed for periods of 700 nm and 900 nm. The higher current values are obtained for structures with triangular profile heights of 300 nm and above.

For the entire spectrum (300 nm – 1100 nm) the short circuit current was calculated to be 12.3 mA/cm$^2$, 15.33 mA/cm$^2$ and 18.9 mA/cm$^2$ for the solar cell on smooth substrate, with triangular structures of period 100 nm and 900 nm, respectively. The latter, where the period is in the range of the incoming wavelengths, has the highest short circuit current because it best utilizes the diffraction and scattering of light. The enhancement comes from light trapping of the longer wavelengths. On the other hand, with a texture period of 100 nm, the small gain in short circuit current is due to its better incoupling of the shorter wavelengths into the cell.

5.3 Parasitic Absorption Losses

As seen from the previous section, the short circuit current is maximized for periods in the range of the incident wavelength and for heights of 400 nm or above. In order to further increase the short circuit current of the solar cell the optical losses have to be minimized. Parasitic absorptions in the front zinc-oxide layer, p-layer of the p-i-n diode and at the back n-layer and zinc-oxide do not contribute to the overall short circuit current. In Fig. 5.6, the quantum efficiency in the i-layer of the silicon diode is shown along with the parasitic absorptions in the p-layer of silicon and the transparent conductive oxide front contact. The absorption in the microcrystalline silicon n-layer and the zinc oxide layer in the back is very low, accounting for a loss of less than 2-3%. Moreover, since we assumed a perfect back reflector, the loss in the back contact is zero. Therefore, these losses are not shown in the figure. The thickness of the p-layer silicon was assumed to be 30 nm. Fig. 5.6 shows the absorption in different regions of the solar cell with a period of 700 nm and triangular groove height of 400 nm.

From the quantum efficiency plot shown in Fig. 5.6, the total short circuit current was calculated to be 20 mA/cm$^2$ compared to a short circuit current of 12.3 mA/cm$^2$ for a smooth substrate. In terms of the parasitic absorptions, the p-layer and the front zinc oxide layer, both absorb 10% and 30% respectively of the total absorbed light in the entire solar cell stack. The largest loss in the p-layer is observed for the shorter
Figure 5.6: External quantum efficiency of the 1000 nm thick p-i-n microcrystalline silicon solar cell and parasitic absorptions in the silicon p-layer and front zinc oxide layer. Period and height of the triangular texture were 700 nm and 400 nm, respectively. The absorptions in the n-layer silicon and back zinc oxide are not shown since they are almost negligible.

wavelengths (from 300 nm to 500 nm), whereas the layer is almost transparent for the longer wavelengths. Absorption loss in the front zinc oxide layer for shorter wavelengths accounts for almost 50%. For wavelengths ranging from 500 nm to 750 nm, the absorption in the front zinc oxide is minimized. Optical loss in the aluminum-doped front zinc oxide layer for longer wavelengths increases as a result of the free carrier absorption. From Fig. 5.6, information on the total reflection of the solar cell structure can also be extracted. The reflection can be simply calculated by \( R = 1 - A \), where \( A \) is the total absorption of the solar cell. The white area in Fig. 5.6 represents the total reflection from the solar cell. It can be observed that for the longer wavelengths, a major portion of the incident energy is lost as reflection. Our studies on different thicknesses of the i-layer has shown that reduction of the reflection should be the key point in optimizing thinner solar cells. Detailed description of those results are given in Chapter 7.

5.4 Summary

Light trapping and incoupling of light in thin-film microcrystalline silicon solar cells with periodic triangular profiles was investigated. Compared to that of a solar cell
on a smooth substrate with 1 \( \mu \text{m} \) thick absorber layer, the short circuit current and quantum efficiency are enhanced with the introduction of triangular texturing. The degree of enhancement highly depends on the period of the triangular profile unit cell. When periods of the texture are smaller than the incident wavelength, enhancement in the shorter wavelengths (300 – 500 nm) of the spectrum comes as a result of better incoupling of the light into the absorber layer. For longer wavelengths (700 – 1100 nm) the short circuit current is distinctly enhanced if the period of the triangular profile unit cell is in the range of the incident wavelength. Along with the period, combination of the period and height of the triangular unit cell is also important. Optimal dimensions were found to be for combinations of the triangular profile where the opening angle of the triangle is equal or close to 90°. The total short circuit current for the entire spectrum is increased from 12.3 mA/cm\(^2\) by 60% up to 20 mA/cm\(^2\) for the best case triangular profile (period of 700 nm and height of 500 nm).
Chapter 6

Simpler and Faster Method for Periodic Textures - using Rigorous Coupled Wave Analysis

In this chapter, a simple and fast method was developed to determine the optimal surface texture of thin-film silicon solar cells. Inline with the results from the previous two chapters, the optical wave propagation was studied for microcrystalline thin-film silicon solar cells with integrated line and triangular gratings. For such periodic surface texture, Rigorous Coupled Wave Analysis (RCWA) provides a faster method in solving the Maxwell’s equations. The method facilitates an analysis of nanotextured solar cells which is 20 times faster than conventional approaches like Finite Difference and Finite Integral simulations. The quantum efficiency curves calculated using RCWA provided a good agreement with experimental data. Moreover, a simplified approach of analyzing optical performance of texture etched solar cells are also discussed.

6.1 Optical Simulation Model

In order to derive the optimal dimensions of nanotextured thin-film silicon solar cells, rigorous calculations to solve the Maxwell’s equations are necessary. If these nanotextured surfaces are periodic, which is the case for theses studies in this thesis, Rigorous Coupled Wave Analysis (RCWA) can solve the electromagnetics equations with much lower computational complexity. To date, most reported works have commonly utilized finite difference time domain (FDTD) method, finite element method (FEM), or finite integration technique (FIT). By using these techniques the influence of the nanotexture on the absorption, quantum efficiency, and short circuit current was investigated for amorphous, microcrystalline, and crystalline silicon solar cells. [9–11, 98, 100, 103, 115] Even though these methods provide a detailed analysis of the
absorption in individual layers of the device, the time complexities for these algorithms are very high. The Rigorous Coupled Wave Analysis, on the other hand, provides an alternative and significantly faster approach to simulate the diffraction and scattering in a nanotextured thin-film solar cell. The working principle of the RCWA algorithm was briefly presented in section 3.3.2 on page 40. Historically, RCWA was first developed to simulate the optics of diffraction gratings [78, 88]. For crystalline silicon solar cells, where it does not have multiple absorbing layers, the quantum efficiency can be calculated by simply subtracting the reflection from the total incident light [116]. However, the RCWA method does not provide the absorption in the individual layers of the device structures. It determines the transmission and reflection of the grating structure for different diffraction orders. In this chapter a method was developed that allows for determining the quantum efficiency and short circuit current based on the reflection and transmission data one obtains from the analysis using RCWA.

A schematic diagram of the solar cell with randomly textured interfaces is shown in Fig. 6.1(a). Since the understanding of the wave propagation in a randomly textured solar cell is complex, a solar cell with periodic texture was investigated to compare the simulations with experimental results. Similar to the schematic in Fig. 6.1(b),

Figure 6.1: Schematic cross sections of a microcrystalline thin-film silicon solar cell with an integrated surface texture. (a) As-deposited solar cell with randomized textured interfaces. (b, c) Unit cell of the periodic arrangement used in this study, where the surface texture was approximated with an integrated line grating and triangular grating, respectively.
6.1. Optical Simulation Model

Microcrystalline silicon solar cells with integrated line grating were prepared experimentally (Ref. [108]). The experimental results were compared to the calculated results from this study. The line grating structure can be described on the basis of the grating period and height of the surface texture. Keeping consistency with the studies from the previous two chapters, the silicon solar cell structure consists of a 500-nm-thick aluminum-doped zinc oxide (ZnO:Al) front contact, followed by a 1000 nm hydrogenated microcrystalline p-i-n silicon diode. The back reflector of the solar cells consists of an 80-nm-thick ZnO:Al layer and a perfect metal reflector (material with a high extinction coefficient). Conformal deposition of the microcrystalline p-i-n solar cell on top of the nanotextured front contact ensures that the texturing extends all the way through the layer stack. There is one notable difference in the optical model compared to the models presented in chapters 4 and 5. Since the RCWA algorithm could only handle a two-material system in its discretized layer stacks, the back contact of the solar cell design had to be slightly modified. In the line grating structure [Fig. 6.1(b)], there was no 80 nm thick back zinc-oxide layer on the vertical boundaries of the back grating. And the back zinc-oxide had to be totally ignored for the triangular textured case [Fig. 6.1(c)]. Despite these small changes, the results from FDTD based simulations and RCWA provided a very good match. The unit cell was illuminated under normal incidence.

6.1.1 Calculation of Quantum Efficiency from RCWA Method

The Rigorous Coupled Wave Analysis allows only for determining the transmission and reflection of the different diffraction orders. By varying the period and height of a grating, the desired diffraction orders can either be enhanced or suppressed. An illustration of the transmission and reflection properties of a grating with period of 700 nm for varying heights of the grating were shown in Fig. 4.6 on page 51 and Fig. 4.7 on page 52. In order to calculate the absorption in the individual layers of the solar cells, an approach based on the transfer matrix method was developed. The transfer matrix elements are determined by carrying out simulations for individual layers of the solar cell. In the case of a microcrystalline thin-film silicon solar cell, the parasitic absorbance is largely determined by the absorption of light in the front ZnO:Al layer and p-layer of the p-i-n solar cell. The absorptions of the n-layer and rear ZnO:Al layer are very low. Hence, the influences of the n-layer and rear ZnO:Al layer were ignored in this model for simplicity. In order to calculate the quantum efficiency of the solar cell, two separate simulations had to performed first with different optical data for the materials in the thin-film solar cell. In the next step, the results from the two simulations were utilized to calculate the absorption in the i-layer of the silicon solar cell. The different steps of this calculation are shown in Fig. 6.2. Along with the
schematic diagrams for the setup of the simulations, the corresponding resulting curves are also shown on the right hand side of the figure. As an illustration, the calculation procedure for the quantum efficiency of a solar cell with a line grating of period 700 nm and height of 300 nm is shown.

The first step (Fig. 6.2) involves calculating the absorption in the parasitic front layer consisting of the stack of zinc-oxide and p-Si layer. By setting the extinction coefficient of an infinitely thick silicon absorber layer to zero \( (\kappa_{Si} = 0) \), the reflection from the stacked layers and the transmission through inside the silicon layer was calculated. Using the conservation relationship of \( (\text{Absorption + Transmission + Reflection} = 1) \) for this stacked structure, we can calculate the absorption in the zinc-oxide and p-Si layer. For the purpose of calculating the final quantum efficiency inside the silicon i-layer, the value of \( 1 - A_{\text{Front}}(\lambda) \) is of more interest. The value excluding the parasitic absorption at the front contact, \( A_{\text{Front}}(\lambda) \), can be expressed as

\[
1 - A_{\text{Front}}(\lambda) = [R_{\text{Front}}(\lambda) + T_{\text{Front}}(\lambda)]
\]  

(6.1)

where \( R_{\text{Front}} \) and \( T_{\text{Front}} \) are the reflectance and transmission, respectively, of the front layer structure (zinc-oxide layer and the p-Si layer).

In the second step, the reflection from an entire solar cell stack without any parasitic front absorption was calculated. Similar to step one, this was achieved by setting the extinction coefficient of the front stacks to zero \( (\kappa_{\text{Front}} = 0) \). Thus the (overestimated) absorption at the silicon absorber layer can be expressed as

\[
A_{\text{Si}}(\lambda) = [1 - R_{\text{Cell}}(\lambda)]
\]  

(6.2)

where \( R_{\text{Cell}} \) is the total reflection of the entire solar cell stack (see Fig. 6.2 step 2). Subsequently, the external quantum efficiency \( EQE(\lambda) \) can be calculated as

\[
EQE(\lambda) \approx [R_{\text{Front}}(\lambda) + T_{\text{Front}}(\lambda)] \cdot [1 - R_{\text{Cell}}(\lambda)] \cdot IQE(\lambda)
\]  

(6.3)

where the absorption of the solar cell without any parasitic front absorption \( A_{\text{Si}} \) (from Eq. 6.2) is corrected using the term \( 1 - A_{\text{Front}}(\lambda) \)(from Eq. 6.1). Furthermore, it was assumed that the internal quantum efficiency, \( IQE(\lambda) \), is equal to unity, which is a good approximation for such thin solar cells [117].
Figure 6.2: The 3 steps in calculating the external quantum efficiency inside the silicon i-layer of a multi layered thin film silicon solar cell. Resulting curves from each step are shown on the right hand side plots. Illustrated is a case for a line grating with period 700 nm and height of 300 nm.
6. Simpler and Faster Method for Periodic Textures - Using Rigorous Coupled Wave Analysis

6.2 Results and Discussion

6.2.1 Comparison of Optical Simulations and Experimental Results

In order to verify the calculated $EQE(\lambda)$ in Eq. 6.3, the experimentally obtained quantum efficiencies of a 1 $\mu$m-thick microcrystalline silicon thin-film solar cell were compared with the calculated quantum efficiencies. Prototype solar cells with integrated line gratings were used as a benchmark to test the developed approach. The measured quantum efficiencies of fabricated solar cells on a smooth substrate [Fig. 6.3(a)] and with an integrated line grating [Fig. 6.3(b)] are shown in Fig. 6.3. The grating period is equal to 1.2 $\mu$m, while the grating height is equal to 300 nm. Compared with the quantum efficiency of the solar cell on a smooth substrate, a distinct increase in the quantum efficiency in the red and infrared parts of the optical spectrum is observed with the introduction of the line grating. The quantum efficiencies in the blue and green parts of the optical spectrum remain almost unchanged by the line grating, since the blue and green lights are absorbed within the first few hundred nanometers of the solar cell. The total short circuit current under AM 1.5 sun spectrum is enhanced by 40% from 12.5 up to 17.3 mA/cm$^2$.

The simulated quantum efficiencies on smooth and textured substrates are also shown in Fig. 6.3. A good agreement between the measured and simulated quantum efficiencies was observed. The thickness of the p-layer of the simulated microcrys-
talline silicon p-i-n solar cell was assumed to be 30 nm. Since the shorter wavelengths (from 300 - 500 nm) are absorbed within one pass of the solar cell, almost identical curves for the simulated and measured quantum efficiencies in this spectral region are observed. For longer wavelengths, the quantum efficiency is increased due to the efficient scattering of light by the front and back gratings. For a grating period of 1200 nm and height of 300 nm, most of the light in the red part of the spectrum (wavelength 500 - 800 nm) is diffracted by the front grating in the 0\textsuperscript{th} order, and for wavelengths in the infrared part of the spectrum (wavelength 750 - 1100 nm), the waves are diffracted in higher diffraction orders. The light that directly reaches the back contact (0\textsuperscript{th} order front grating) is efficiently diffracted by the back grating into higher diffraction orders, thus allowing most of the light to be absorbed in the solar cell. The sharp interference fringes of the calculated quantum efficiencies, which are visible in Fig. 6.3, are caused by the interference of the backward and forward propagating light. The quantum efficiency was calculated for monochromatic light, whereas the experimental data was measured using a spectrometer with a spectral width of 15 nm; consequently, the interference fringes of the experimental measurement are less pronounced and appear to be smoother.

6.2.2 Optical Performance of Solar Cells with Integrated Line and Triangular Gratings

After initial verification of the developed approach by comparing it with experimental results, the RCWA method was utilized to sweep the varying period and height of integrated line and triangular textures in a solar cell. In terms of the simulations performed, the period of the interface texture was varied from 0 to 3000 nm at an interval of every 100 nm and the height of the texture was varied in the range of 0 to 500 nm by 20 nm steps. Since the computational complexity of the RCWA method compared to FDTD solvers was much lower, it allowed us to sweep the varying period and height of the texture with more precision, which was not previously possible.

The influence of the grating period and the grating height on the short circuit current is shown for a solar cell with a line [Figs. 6.4(a)-6.4(c)] and a triangular grating [Figs. 6.5(a)-6.5(c)]. The triangular grating, as shown in Fig. 6.1(c), was investigated as an improvement of the line grating structure since it resembles the randomly textured surface more accurately. The calculated short circuit current is shown in Figs. 6.4(a) and 6.5(a) under blue (wavelength 300 – 500 nm) illumination and in Figs. 6.4(b) and 6.5(b) under red and infrared (wavelength 700 – 1100 nm) illumination. The short circuit current of the solar cell under AM 1.5 illumination (wavelength 300 – 1100 nm) is given in Figs. 6.4(c) and 6.5(c).

Irrespective of the dimension of the grating height, an increase in the short circuit
Figure 6.4: Short circuit current for a 1-µm-thick microcrystalline silicon solar cell as a function of the grating period and height illuminated under (a) blue light (wavelength 300 – 500 nm), (b) red and infrared light (wavelength 700 – 1100 nm), and (c) entire sun spectrum (wavelength 300 – 1100 nm). The set of figures show the behavior of solar cells with integrated line grating.

Current compared with that of the flat case is observed. When illuminated by an AM 1.5 sun spectrum [Figs. 6.4(c) and 6.5(c)], the maximum short circuit current is observed for grating periods of approximately 500 - 700 nm. Compared with the short circuit current of a solar cell on a smooth substrate, the short circuit current is increased by around 60% from 13 to 20 and 21 mA/cm² for the line grating and triangular grating, respectively. The behavior of the short circuit current in Figs. 6.4 and 6.5 as a function of the grating period can be explained as follows: For grating periods much smaller than the incident wavelength, only a slight enhancement of the short circuit current is observed for the blue part of the optical spectrum. The enhancement of the short circuit current is caused by an improved incoupling of shorter-wavelength light [Figs. 6.4(a) and 6.5(a)]. Compared with a solar cell on a smooth substrate, an enhancement
Figure 6.5: Short circuit current for a 1-μm-thick microcrystalline silicon solar cell as a function of the grating period and height illuminated under (a) blue light (wavelength 300 – 500 nm), (b) red and infrared light (wavelength 700 – 1100 nm), and (c) entire sun spectrum (wavelength 300 – 1100 nm). The set of figures show the behavior of solar cells with triangular grating.

of around 1 mA/cm$^2$ is observed. This enhancement of the short circuit current is observed for grating periods smaller than 300 nm. Since the period of the grating is smaller than the incident wavelength, the grating acts as an effective refractive index gradient. The graded refractive index acts as a matching layer between the refractive index of zinc oxide and microcrystalline silicon. For grating periods larger than the incident wavelengths (period > 1 μm), the short circuit current drops as well. Light is only diffracted at small diffraction angles, which can be explained using the grating equation (Eq. 4.7 on page 55). Henceforth, the diffracted light does not interfere with diffracted light from neighboring unit cells. The intensity profile essentially becomes a superposition of absorption pattern arising from a flat solar cell and that from the grating of the unit cell. Thus, the short circuit current for such large grating periods
converges towards that of a solar cell on a flat substrate.

While the short circuit current of solar cells with integrated line grating drops for grating periods larger than 1 $\mu$m, the short circuit current of solar cells with integrated triangular grating remains high for grating periods up to 3 $\mu$m. In case of the triangular gratings, the variation of the opening angle as a function of the period and height of the grating is shown in Fig. 6.6. If we map the figure to the short circuit current map of Fig. 6.5(c), we can observe that for opening angles up to $120^\circ$, the grating can achieve higher short circuit current. The solar cells with a larger period can still attain higher absorption, provided their groove heights are high as well. The combination of larger grating periods along with high groove heights ensures that the light reflected by the back contact is totally internally reflected to the outside medium/ZnO interface. The opening angle of the triangular texture plays a major role in achieving higher absorptions in the silicon layer. It was previously reported that optimal opening angles of the triangular texture are close to $90^\circ$ [118]. If the grating period is comparable to the incident wavelengths, the diffraction angles are large enough for the diffracted waves to propagate into neighboring unit cells. Diffracted waves can thus interfere constructively or destructively within the thin absorber layer. Interaction of these waves contributes to the higher short circuit current under red and infrared illumination (wavelength 700 – 1100 nm) that is observed for grating periods around 700 nm [Figs. 6.4(b) and 6.5(b)]. The highest short circuit current is observed for grating
6.2. Results and Discussion

Figure 6.7: Discretization of the 1-dimensional AFM line scan into layered stacks in order to analyze the surface using the RCWA method. Each layer stack was 10 nm thick.

heights of 350 to 400 nm for line grating and around 450 to 500 nm for triangular grating. A comparison of the contour map in Figs. 6.4(b) and 6.5(b) with Figs. 6.4(c) and 6.5(c) shows that the gain of the total short circuit current under AM 1.5 illumination is dominated by the efficient diffraction of the longer-wavelength light. Furthermore, a comparison of the calculated currents with that obtained from Finite Difference Time Domain simulations exhibits a very good agreement. Only for the longer wavelengths, Equation 6.3 slightly overestimated the quantum efficiency. The error was calculated to be smaller than $\pm 1.5 \text{ mA/cm}^2$.

6.2.3 Analyzing Texture Etched Substrates

As discussed in the previous chapters, one of the most commonly used method for achieving higher short circuit current is by etching the sputtered zinc-oxide layer in a dilute HCl acid. In order to fully analyze the optical properties of such randomly textured substrates and study its influence on the overall short circuit current, 3-dimensional simulations of large scan areas are necessary for an accurate representation. But if we allow ourselves to break the randomized problem into a 1-dimensional line scan, we can utilize the RCWA method to study the trends in the quantum efficiency and short circuit current for different texture etched zinc-oxide substrates. Assuming a line scan from an AFM scan of a randomly textured zinc-oxide can be represented as a periodic texture, the discretization of the line scan for using with the
Figure 6.8: Calculated quantum efficiency of solar cells deposited on a line scan of the textured zinc-oxide substrates etched for 5, 15 and 20 sec. The solar cell on a smooth substrate is also shown as a reference.

RCWA method is shown in Fig. 6.7. Depending on the height variation of the textured substrate, different thicknesses of the layer stacks were chosen such that the error due to discretization is minimal. In case for the Fig. 6.7, layer stacks with thicknesses of 10 nm are shown.

Following the discretization of the AFM line scans, the quantum efficiency for solar cells deposited on the textured line scans can be calculated using Eq. 6.3. Due to the randomized nature of the line scans, incorporating the p-Si layer on the solar cell stack was not trivial. Hence, the calculated quantum efficiencies in this section included the absorption in the parasitic p-layer of the silicon diode. While this parasitic absorption has a big influence in the shorter wavelength spectrum ($\lambda < 500$ nm), its influence on the longer wavelength region ($\lambda > 600$ nm), where light trapping effects due to texturing kicks in, is very small. The calculated quantum efficiencies for solar cells on a smooth substrate and textured zinc-oxide substrates etched for 5, 15 and 20 seconds are shown in Fig. 6.8.

It can be observed that the interference fringes similar to the quantum efficiency curve from solar cell on a smooth substrate is visible for the solar cells on textured substrates as well. From experimentally measured quantum efficiency curves, one would assume that these fringes should smoothen out as the substrate is made rough from the texturing. But since in the calculation based on RCWA, the random AFM line scans were periodic for every 5 $\mu$m length, the fringes do not disappear completely.
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Figure 6.9: Calculated short circuit current gain relative to that from a solar cell on a smooth substrate. Cases for 3 different substrates etched for 5, 15 and 20 seconds are shown.

Moreover, experimental data are measured using a spectrometer with a spectral width of 15 nm. Thus the interference fringes of experimental quantum efficiency curves are less pronounced and appear to be smoother. In order to compare the different series of quantum efficiencies, the short circuit current obtained from these curves were calculated using Eq. 4.5 on page 54. For the solar cell on a smooth substrate, short circuit current of 15.63 mA/cm$^2$ was calculated. The main objective of this part of the study was not to calculate the absolute numbers for the achievable short circuit current, but to rather predict how it changes with varying etching time of the zinc-oxide substrate. The relative gain of the short circuit current with respect to that from a solar cell on a smooth substrate is shown in Fig. 6.9. The bar plot shows the relative gain for the solar cells under AM 1.5 illumination ($\lambda = 300 - 1100$ nm) and under red illumination ($\lambda = 700 - 1100$ nm). The trend observable from Fig. 6.9 is consistent to expectations from what is observed in experimental results [119]. With increasing surface roughness due to texturing, increase of the total short circuit current is seen. Moreover, the gain in the red current highlights the light trapping effects due to surface texturing. Even though the gain in the red current for substrates etched under 20 seconds was lower compared to the gain for total current, more than 20% gain was achieved for the zinc-oxide substrate etched for 20 seconds. Thus, by simplifying the random textured substrates into a 1-dimensional line scan, the optical performance for
different texture series can still be analyzed using RCWA method.

6.3 Summary

A simple and very fast method was developed to optimize the short circuit current of nanotextured thin-film solar cells. The Rigorous Coupled Wave Analysis was used to analyze the optical wave propagation in microcrystalline thin-film silicon solar cells with line and triangular gratings. The simulation results are in good agreement with the results obtained from experimental data. RCWA facilitates a distinctly faster analysis of the optics in nanotextured thin-film solar cells compared with conventional full-wave electromagnetic simulations. The short circuit current for 1-μm-thick microcrystalline silicon solar cells with surface texture is maximized if the texture period is close to 700 nm. Compared to the solar cells with integrated line grating, the performance of solar cells with triangular texture is less affected by variations of the texture period and height. Even for larger periods, if the texture height is high enough, such that the opening angle of the texture is less than 120°, the performance of the triangular texture does not suffer. Applications of RCWA for analyzing randomly textured substrates were discussed. The calculated trend of the short circuit current reveals that such analysis would be helpful in optimizing the optical properties of texture etched zinc-oxide substrates.
Chapter 7

µc-Si Solar Cells with 3-dimensional Surface Texture

Until now, the influence of surface texture on the solar cell optical properties were investigated using 2-dimensional simulations. In this chapter, the optical enhancement and losses of microcrystalline thin-film silicon solar cells were investigated for 3-dimensional surface texture. Using a finite difference time domain algorithm, the influence of the profile dimensions (the period and height of the pyramid) and solar cell thickness on the quantum efficiency and short circuit current were analyzed. Furthermore, the influence of the solar cell thickness on the upper limit of the short circuit current was investigated. The numerically simulated short circuit currents were compared to fundamental light trapping limits based on geometric optics. The theoretical light trapping model is based on the original work by Yablonovitch and Cody [67]. Yablonovitch and Cody derived an upper light trapping limit based on geometric optics. In this study, the model was extended, taking unavoidable optical losses in the solar cell into account. Finally, optical losses in the solar cell were analyzed. After identifying these key losses, strategies for minimizing the losses were discussed.

7.1 Optical Simulation Model

One of the primary aims when optimizing thin-film solar cells is to increase the absorption of the solar cell. Different strategies, which includes using anti-reflection coatings [96], optical filters [98], or highly reflective back contacts [120], have been widely investigated and used in research. In the case of microcrystalline thin-film silicon solar cells, randomly textured contact layers have so far resulted in the highest short circuit currents [6, 23]. Solar cells with textured contact layers can be realized by growing the solar cell directly on either a textured back (n-i-p solar cell) or front (p-i-n solar cell) contact. Textured and transparent contact layers can be fabricated by the direct
growth of zinc oxide films via low pressure chemical vapor deposition (LPCVD) or the etching of sputtered zinc oxide [110, 119]. A schematic cross section of a randomly textured solar cell is shown in Fig. 7.1(b). Understanding and optimizing the wave propagation in solar cells with randomly textured contact layers is complex. Depending on the experimental technique used to fabricate the nanotextured contact, the films exhibit a pyramid- or a crater-like texture. Zinc oxide films prepared via LPCVD exhibit a pyramid-like texture, whereas films prepared via sputtering and subsequent etching show a crater-like texture [31, 119, 121]. Commercially available tin oxide films (e.g., Asahi-U substrates) also have a pyramid-like texture [59]. The random surface texture was approximated using a periodic arrangement of light trapping structures. So far the optical simulations were carried out for 2-dimensional structures. In the following the behavior of 3-dimensional pyramid- or crater-like textured substrates will be investigated. The 3-dimensional surface texture is represented by arrays of square based pyramid structures that are periodic in both the x- and y- direction. By simulating the optics in three dimensions, the wave propagation in the textured solar cells was studied.

Previous investigations of Haase and coworkers show that random surface textures can be approximated by periodic surface textures [122]. They studied the optical wave
propagation of light in microcrystalline silicon thin-film solar cells on quasi-random surfaces. Such surfaces consist of a large number of randomly arranged pyramids. The short circuit current of the solar cell on the quasi-random surfaces was calculated and compared to simulations of periodic surface textures. The short circuit current of the solar cell on the quasi-random surface could be determined by an area weighted superposition of the short circuit current for periodic surface textures. These simulation results indicate that for thin-film solar cells based on amorphous or microcrystalline silicon, the optics of randomly textured substrates can be approximated by the area weighted superposition of optical simulations of periodic structures.

The cross sections of a solar cell deposited on a smooth substrate and a pyramid texture are shown in Figs. 7.1(a) and 7.1(c). The cross section of the pyramid textured solar cell is taken in the middle of the unit cell; therefore it resembles a triangle-like texture. The microcrystalline silicon solar cell structure consists of a 500 nm thick aluminum doped zinc oxide (ZnO:Al) front contact deposited on a thick glass substrate. The zinc oxide layer is followed by a (p-i-n) hydrogenated microcrystalline silicon diode (µc-Si:H) with a total thickness of 0.5 to 3.5 µm and a back contact consisting of an 80 nm thick ZnO:Al layer and a perfect metal back reflector. The p-layer of the solar cell was assumed to be 30 nm thick. The device structure is consistent with standard microcrystalline silicon solar cells prepared by several research groups [93, 95]. The period of the unit cell was varied from 50 nm to 6000 nm, and the pyramid height was varied from 100 nm to 500 nm. The unit cell was illuminated under normal incidence using a standard AM 1.5 sun spectrum. The input wave for the simulations was assumed to be circularly polarized.

7.2 Simulation Results

7.2.1 Solar Cells with Textured Interfaces

The quantum efficiency and short circuit current were utilized in order to compare the solar cells with different surface textures. From the electric fields exported from the 3-dimensional simulations, the power loss was calculated using the equation

\[ Q(x, y, z) = \frac{1}{2} \varepsilon_0 n \alpha \left| E(x, y, z) \right|^2 \]  \hspace{1cm} (7.1)

where \( c \) is the speed of light in free space; \( \varepsilon_0 \) is the permittivity of free space; \( \alpha \) is the energy absorption coefficient (\( \alpha = 4\pi k / \lambda \)), with \( n \) and \( k \) being the real and imaginary parts of the complex refractive index; \( \lambda \) is the wavelength; and \( E \) is the electric field. The power loss profile under blue (\( \lambda = 400 \) nm) and red (\( \lambda = 700 \) nm) illumination is shown in Fig. 7.2.
The period and height of both of the pyramid textures were 700 nm and 400 nm, respectively. The thickness of both of the microcrystalline silicon diodes was 1 µm. The wavelengths of the incident light were 400 nm and 700 nm. Shorter wavelengths (λ =400 nm) get absorbed within the first 200 nm of the solar cell. The power loss pattern is shown in Fig. 7.2(a). With increasing wavelength, the photons penetrate deeper in the microcrystalline silicon absorber. Due to the low absorption coefficient of microcrystalline silicon for longer wavelengths, light has to complete multiple passes in the thin microcrystalline silicon solar cell before it is completely absorbed. The power loss profile for red illumination (λ =700 nm) is shown in Fig. 7.2(b). The incoming light reaches the back contact of the solar cell, where it gets reflected and completes multiple passes within the solar cell. Because the opening angle of the pyramid texture is close to 90°, the absorption of light close to the back reflector is high as shown in Fig. 7.2(b) [118]. In the next step, the quantum efficiency and the short circuit current were calculated. The quantum efficiency is defined as the ratio of the power absorbed in the intrinsic microcrystalline silicon absorber to the total power incident on the unit cell. The following relation was used to calculate the quantum efficiency:

\[
QE = \frac{1}{P_{opt}} \int Q(x, y, z) dx dy dz
\]  

(7.2)
7.2. Simulation Results

Figure 7.3: Short circuit current map for a 1 µm thick microcrystalline silicon solar cell as a function of the period and height of the pyramidal unit cell. The solar cells were illuminated under AM 1.5 sun spectrum (wavelength 300-1100 nm)

where \( Q(x, y, z) \) is the time averaged power loss and \( P_{opt} \) is the optical input power. The internal quantum efficiency is assumed to be 100%. Therefore, the results present an upper limit of the external quantum efficiency and short circuit current. Based on the quantum efficiency, the short circuit current can be calculated:

\[
I_{SC} = \frac{q}{hc} \int_{\lambda_{min}}^{\lambda_{max}} \lambda Q E(\lambda) S(\lambda) d\lambda
\]  

(7.3)

where \( q \) is the elementary charge, \( \lambda \) is the wavelength, \( h \) is Planck’s constant, \( c \) is the speed of light, and \( S(\lambda) \) is the weighted sun spectrum (AM 1.5 spectral irradiance). The influence of the dimensions of the pyramidal texture on the short circuit current is presented in Fig. 7.3.

The short circuit current map is shown as a function of the period and height of the square based pyramidal unit cell. The highest current is achieved for periods between 700 nm and 1500 nm and for profile heights of 400 nm and 500 nm. Compared to the short circuit current on a smooth substrate, the maximum short circuit current of 22.5 mA/cm\(^2\) is achieved with an increase of 84% from 12.25 mA/cm\(^2\). For smaller periods (<300 nm), only a slight improvement in the short circuit current due to better incoupling of the shorter wavelengths (wavelength 300 to 500 nm) is observed. While light trapping does not have a significant effect on the short circuit current for
short wavelengths, it has a major impact for longer wavelengths. Light is efficiently
diffracted and scattered by the pyramid texture, resulting in an enhanced short circuit
current. From the grating equation (Eq. 4.7 on page 55), we know that with increasing
period of the grating, the diffraction angle is reduced. Consequently, the diffracted
higher orders do not interfere with the diffracted orders from the neighboring unit
cell. The constructive interference of the diffracted orders is essential for efficient light
trapping in the solar cell. Hence the short circuit current for periods larger than the
incident wavelengths (period > 3 \( \mu m \)) converges toward that of a solar cell on a flat
substrate. When the texture period is comparable to the incident wavelength (e.g.,
a pyramid period of 700 nm to 1200 nm), diffracted waves of neighboring unit cells
constructively interfere, resulting in a higher short circuit current.

**2D Versus 3D Texture**

Compared to the total short circuit values obtained for solar cells with 2-dimensional
triangular texture in chapters 5 and 6, the current values in Fig. 7.3 calculated from
square based pyramids are higher by more than 2 mA/cm\(^2\). This increase is a conse-
quence of introducing the third dimension which allows additional optical diffraction
in that plane to happen. A comparative quantum efficiency plots for solar cells with
triangular texture and square based pyramid texture is shown in Fig. 7.4. The period
7.2. Simulation Results

Figure 7.5: Short circuit current (wavelength=300–1100 nm) for different periods of the unit cell as a function of the absorber layer thickness. The pyramid height of all of the textured solar cells was 400 nm. The dashed line represents the short circuit current for a solar cell on a smooth substrate.

and height of the surface texture were 900 nm and 400 nm, respectively. The quantum efficiency of a solar cell on a smooth substrate is also shown as a reference. For wavelengths shorter than 450 nm, there is no significant difference between the 2D and 3D case. This effect is not pronounced in the blue part of the spectrum since incoming light at this wavelengths gets absorbed within the first 200 nm of the absorber layer and the addition of a diffraction plane does not contribute to better absorption. For the longer wavelength region (λ > 600 nm), the additional diffraction plane leads to a clearly enhanced quantum efficiency for the 3D textured case compared to the triangular texture. Enhancement of more than 100% was achieved at wavelength 720 nm. Thus in order to design optimal light trapping structures, such enhancements as observed by introducing additional diffraction plane are very significant. In terms of the calculated short circuit current, a gain of 3.7 mA/cm² was obtained for the pyramid textured case compared to 18.12 mA/cm² calculated for the triangular textured solar cell.

Influence of Absorber Layer Thickness

Up to this point, the thickness of the microcrystalline silicon diode was kept constant at 1 µm. The influence of the absorber layer thickness on the short circuit current
is shown in Fig. 7.5. The thickness of the microcrystalline silicon diode was varied from 0.5 \( \mu \text{m} \) to 3.5 \( \mu \text{m} \). The short circuit current was calculated for structures of three different periods. The height of the pyramid texture was kept constant at 400 nm, and periods of 700 nm, 900 nm, and 1200 nm were investigated. The dashed line represents a solar cell on a smooth substrate.

As the thickness of the solar cell is increased, a significant increase of the short circuit current can be observed for all three grating periods. In the case of a 700 nm period, an increase of 106% in the short circuit current was obtained from 9.07 mA/cm\(^2\) to 18.71 mA/cm\(^2\), for a silicon diode layer thickness of 0.5 \( \mu \text{m} \). For a solar cell thickness of 3.5 \( \mu \text{m} \), the short circuit increases from 20.35 mA/cm\(^2\) to 25.85 mA/cm\(^2\). With increasing thickness of the absorber layer, the relative gain in the short circuit current due to the surface texture is reduced.

### 7.2.2 Limits of the Short Circuit Current

The idea of using light trapping to enhance the total absorption in thin films has been studied for more than four decades. Yablonovitch and Cody were the first to determine an upper geometric light trapping limit [22, 123]. They showed that the light intensity in a thin film with perfect surface texturing can be enhanced by \( 2n^2 \), where \( n \) is the real part of the complex refractive index of the thin film. In the case of microcrystalline silicon with a refractive index of 3.6, the light bounces back and forth 25 times as compared to a thin film without a surface texture. A perfect surface, in this case, means that the surface is textured in such a way that the reflection is zero (R=0), so that all light enters the structure. The intensity within a thin film with an ideal surface texture and a back reflector with a reflectivity of 100% is enhanced by \( 4n^2 \).

Based on the work of Yablonovitch and Cody, the absorption in such a thin film with a perfect front texture and a perfect reflector can be described by

\[
A_{\text{Limit}} = 1 - \exp \left( -4n^2\alpha L \right) \tag{7.4}
\]

where \( A_{\text{Limit}} \) is the absorption limit, \( \lambda \) is the wavelength dependent absorption coefficient of the film, and \( L \) is the thickness of the absorber layer. In comparison, the absorption of a thin film without a light trapping structure is described by the following relation:

\[
A_{\text{NoLT}} = 1 - \exp \left( -2\alpha L \right) \tag{7.5}
\]

The concept of Yablonovitch and Cody was applied to microcrystalline thin-film silicon solar cells. Based on Eq. 7.4, an upper limit of the short circuit current of 36.76 mA/cm\(^2\) for a 1 \( \mu \text{m} \) thick silicon solar cell can be derived. The short circuit current
value represents an upper limit that cannot be achieved due to optical losses and inefficient light incoupling and light trapping. Different models have been suggested that account for some of the optical losses, such as absorption in the front and the back contacts [32, 124]. The models provide valid information about the achievable upper limit of the short circuit current. However, the models rely on experimental input parameters such as the absorption in the front and back contacts. Several authors carried out optical measurements of individual layers, such as the front or the back contact, in order to determine the absorption in those layers [32, 54, 125]. However, measurements of textured front or back contacts cannot be used to approximate the behavior of the same films in a solar cell. The measurements of the individual films were carried out in air, whereas the same films as part of a solar cell are surrounded by different dielectric media. Therefore, a simpler optical model was modeled in order to account for some of the losses in a thin-film solar cell. This model does not rely on the optical measurements of textured layers.

Most of the microcrystalline silicon solar cells are realized in a superstrate configuration. Light enters the solar cell through a glass substrate that is coated by a transparent conductive oxide (TCO). The first and the second interface of the solar cell are flat, which leads to unavoidable reflection losses of the incident light. In the optical simulations, the reflections at the air–glass and glass–ZnO interfaces are taken into consideration. In addition to the reflection of the front surface, the absorption in the front contact has a distinct influence on the absorption of light in the p-i-n microcrystalline thin-film silicon solar cell. In the case of a microcrystalline thin-film silicon solar cell, the front contact usually consists of a 500 nm thick zinc oxide film in order to allow for a sufficient lateral conductivity of the front contact [29]. When calculating the absorption in the zinc oxide layer, a single pass of the light through the ZnO film was assumed, which is given by 

\[
A_{ZnO} = 1 - e^{-\alpha_{ZnO}L_{ZnO}}
\]

where \( L_{ZnO} \) and \( \alpha_{ZnO} \) are the thickness and the absorption coefficient of the ZnO film, respectively. Furthermore, it was assumed that no light is reflected at the ZnO–silicon interface \( (R_{ZnO/Si} = 0) \), so that all of the light enters the microcrystalline silicon p-i-n diode. As a result, the absorption of the solar cell on a smooth substrate can be calculated by

\[
A_{NoLT_Cell} = (1 - R_{air/glass/ZnO}) \cdot (1 - A_{ZnO}) \cdot (1 - e^{-2\alpha_{Si}L_{Si}})
\]

where \( \alpha_{Si} \) and \( L_{Si} \) are the absorption coefficient and thickness of the p-i-n diode. \( R_{air/glass/ZnO} \) is the total reflection from an air/glass/ZnO layered stack, which was calculated considering multiple reflections for the layered system. A schematic cross section of the solar cell is shown in Fig. 7.6. The cross section highlights the propagation direction of the light inside the solar cell at every interface.
Figure 7.6: Schematic sketch of a simplified microcrystalline silicon thin-film solar cell with (a) smooth interfaces and (b) textured interfaces. The propagation of light through the structures is marked by the directional arrows, and the assumptions on reflection are marked near the corresponding interfaces.

Similar to Eq. 7.6, the upper absorption limit considering the unavoidable absorption and reflection losses is given by

\[
A_{\text{Limit,Cell}} = \left(1 - R_{\text{air/glass/ZnO}}\right) \cdot \left(1 - A_{\text{ZnO}}\right) \cdot \left(1 - e^{-4n^2\alpha_{\text{Si}}L_{\text{Si}}}}\right)
\]  

(7.7)

Hereinafter the absorption limit from Eq. 7.7 is referred to as the Yablonovitch limit. The total short circuit current achievable from a 1 μm thick microcrystalline silicon thin-film solar cell without a light scattering structure [Fig. 7.6(a), calculated using Eq. 7.6] is 16.30 mA/cm², whereas a solar cell with a perfect light scattering structure [Fig. 7.6(b), calculated using Eq. 7.7] exhibits a short circuit current of 33.20 mA/cm². The calculated short circuit current for solar cells with no light trapping (Yablonovitch flat) and with perfect light trapping (Yablonovitch textured) is shown in Fig. 7.7. The upper and lower Yablonovitch limit currents are shown as a function of the solar cell diode thickness, which was varied from 100 nm up to 3 μm. The short circuit current gain for the solar cell with perfect light trapping structure is also shown on the right hand side axis of the figure. While the lower limit of the short circuit current is increasing with increasing thicknesses of the diode, the increase is reaching a steady state for the upper limit of the short circuit current. Theoretically, as the thickness of the absorber
layer reaches infinity \((L_{\text{absorber}} \to \infty)\), the relative gain also approaches towards unity. Thus the potential for light trapping gain is higher for thinner solar cells.

Along with the Yablonovitch limit, the simulated quantum efficiencies for two solar cells of different i-layer thicknesses are shown in Fig. 7.8. The quantum efficiencies were calculated for microcrystalline silicon p-i-n solar cells with diode thicknesses of 0.5 \(\mu\text{m}\) [Fig. 7.8(a)] and 2.5 \(\mu\text{m}\) [Fig. 7.8(b)]. In both simulations, a pyramid texture with period of 1200 nm and a height of 400 nm were used. Only the photons absorbed in the i-layer of the solar cell contribute to the short circuit current. The electron–hole pairs absorbed in the p- and n-layer recombine due to the short carrier lifetime. As a result, the calculated quantum efficiency for shorter wavelengths ranging from 300 nm to 500 nm is lower as compared to the Yablonovitch limit. A detailed analysis of the parasitic optical losses in the p-layer is given in Sec. 7.3 on page 103. It can be seen from Fig. 7.8 that for certain wavelengths, the calculated quantum efficiencies of solar cells on a smooth substrate are higher than the quantum efficiency determined by the modified Yablonovitch limit. This observation does not violate the Yablonovitch limit, as the model relies on geometrical optical effects, and interference effects are not considered. Furthermore, the simulations were carried out for a perpendicular incidence of the light. For a different angle of incidence, the calculated quantum efficiency might be below the Yablonovitch limit [19].
Figure 7.8: A comparison of the quantum efficiency of a solar cell on a smooth substrate with that of solar cells with a pyramid period of 1200 nm and a height of 400 nm. Cases for two different silicon diode thicknesses are shown: (a) a thickness of 0.5 μm and (b) a thickness of 2.5 μm. The Yablonovitch upper and lower limits for both of the thicknesses are also overlaid on the plots.
Table 7.1: A comparison of simulated short circuit current and Yablonovitch limit cases for microcrystalline silicon thin-film solar cells with thicknesses of 0.5 µm and 2.5 µm. The simulated results for a solar cell on a smooth substrate and with a pyramid texture with a period of 1200 nm and a height of 400 nm are tabulated.

<table>
<thead>
<tr>
<th>Solar cell thickness</th>
<th>0.5µm</th>
<th>2.5µm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flat substrate</td>
<td>9.07 mA/cm²</td>
<td>18.93 mA/cm²</td>
</tr>
<tr>
<td>Pyramid textured substrate</td>
<td>18.34 mA/cm²</td>
<td>25.57 mA/cm²</td>
</tr>
<tr>
<td>Yablonovitch flat</td>
<td>12.22 mA/cm²</td>
<td>22.15 mA/cm²</td>
</tr>
<tr>
<td>Yablonovitch textured</td>
<td>30.90 mA/cm²</td>
<td>35.46 mA/cm²</td>
</tr>
</tbody>
</table>

In the case of a 0.5 µm thick solar cell, the red and infrared parts of the spectrum are not utilized efficiently due to the high penetration depth of longer wavelengths. After increasing the thickness to 2.5 µm, a significant increase in the quantum efficiency for the red part of the spectrum (λ = 600 nm to λ = 950 nm) can be noted. The short circuit currents for the two structures are summarized in Table 7.1.

The short circuit current for the solar cells on a smooth substrate is smaller than that for a structure allowing for two passes in the solar cell (Yablonovitch flat). Apart from the parasitic absorption loss in the p-layer of the silicon diode, this can be mainly attributed to the fact that a large fraction of the incident light is reflected at the ZnO–Si interface. In Eq. 7.6 the reflection at this interface is assumed to be zero. The short circuit current in the red and infrared parts of the spectrum (wavelength = 600–1100 nm) for a flat structure is comparable for both thicknesses. In the case of a 0.5 µm thick solar cell with a pyramid texture, the total short circuit current under AM 1.5 illumination increases by 102% as compared to that in a flat solar cell. Based on the Yablonovitch model, an increase in the short circuit current of 153% was obtained. Because the solar cell is very thin, the longer wavelength light cannot be efficiently trapped in the solar cell. When the thickness of the solar cell is increased to 2.5 µm, a gain of 35% is obtained as compared to the theoretical limit gain of 60%. The main loss is observed for shorter wavelengths ranging from 300 nm to 450 nm, where a large fraction of the incident light is lost due to absorption in the p-layer. Furthermore, a certain fraction of the incident light is lost due to inefficient light incoupling in the solar cell. Improvements can be achieved by rigorously engineering the period and heights of the surface texture. Moreover, for the 0.5 µm thick and 2.5 µm thick silicon diodes, losses are also observed for wavelengths longer than 600 nm and 700 nm, respectively. Losses in the red and infrared illumination parts of the optical spectrum are due to the ZnO–Si interface reflection and inefficient absorption of longer wavelengths due to imperfect back contact engineering. Hence a back contact that acts like a perfect
Figure 7.9: A comparison of the quantum efficiency of solar cells with different periods of the pyramid unit cell. For a fixed pyramid height of 400 nm, quantum efficiency plots are shown for solar cell thicknesses of (a) 0.5 µm and (b) 2.5 µm.

Lambertian reflector would randomize the direction of the reflected light further and thus improve the light trapping in the solar cell. Nevertheless, it can be seen in Fig. 7.8 that increasing the absorber thickness leads to significant improvements in the quantum efficiency for longer wavelengths.

The influence of the period of the pyramid texture on the quantum efficiencies of
solar cells with absorber thicknesses of 0.5 µm and 2.5 µm is shown in Fig. 7.9. The pyramid height was kept fixed at 400 nm. Fig. 7.9(a) exhibits the quantum efficiencies of thin solar cells (0.5 µm) with texture periods of 300 nm, 400 nm, and 500 nm. For larger pyramid periods, the quantum efficiency in the red and infrared parts of the optical spectrum starts to drop. The quantum efficiencies of 2.5 µm thick solar cells with pyramid periods of 700 nm, 900 nm, and 1200 nm are shown in Fig. 7.9(b). In both figures, the quantum efficiency of a pyramid with a period of 100 nm is also shown. With such small pyramid periods, the incoupling of light into the solar cell is enhanced, but almost no scattering or diffraction of the longer wavelengths’ light is observed.

For a solar cell with a thick absorber layer [Fig. 7.9(b)], the period of the texture influences the quantum efficiency in different ways. The quantum efficiency ranging from wavelengths 300 nm to 600 nm slightly decreases with an increasing period of the unit cell, whereas a gradual increase of the quantum efficiency is observed with longer wavelengths. The diffraction angle, as discussed in the Eq. 4.7 on page 55, gets smaller with an increasing period of the unit cell. When the absorber layer is thinner than 1000 nm, the light trapping potential of the pyramid texture is reduced if the period of the unit cell is larger than 1000 nm. This means that with increasing solar cell thickness, the optimal period of the surface texture increases, too.

The short circuit current gain in structures of different thicknesses is shown in Fig. 7.10. The short circuit current gain was calculated with respect to the solar cell on a smooth substrate. On the left-hand axis, the normalized gain is shown, and the gain in percentage with respect to the flat solar cell is depicted on the right-hand axis of the figure. In all cases, the relative gain decreases with the increasing thickness of the p-i-n solar cell. This is due to the fact that with greater thicknesses, fewer passes of the light are needed in order for it to be fully absorbed by the solar cells. Therefore, the gain with respect to the solar cell on a smooth substrate drops. In contrast, when the solar cell is thicker, the enhancement gain gets closer to the gain achievable from the Yablonovitch limit.

### 7.3 Optical Enhancements and Losses in the Solar Cell

The influence of a pyramid surface texture on the short circuit current of microcrystalline silicon solar cells with different absorber thicknesses have been investigated. The short circuit current is maximized for a texture period of 700 to 1200 nm and a texture height of 400 to 500 nm. However, the maximal short circuit current is still lower than the Yablonovitch limit. By identifying the key losses in the solar cell structure, one can derive potential strategies to minimize these optical losses. The absorptions in the different layers of the solar cell are shown in Fig. 7.11 for absorber
thicknesses of 0.5 \( \mu \text{m} \) and 2.5 \( \mu \text{m} \). In both cases, a pyramid texture with a period of 1200 nm and a height of 400 nm was used. Light absorbed in the p-layer and the n-layer does not contribute to the overall short circuit current. Only the photogenerated charges in the i-layer contribute to the total short circuit current. The absorption in the individual regions of the microcrystalline diode is shown in Fig. 7.11. A large fraction of the blue light is absorbed in the p-layer. The p-layer thickness was assumed to be 30 nm. Because the absorption in the n-layer is very small, it is not shown in Fig. 7.11.

In Fig. 7.11(a), the quantum efficiency and absorption calculated for a solar cell with a 0.5 \( \mu \text{m} \)-thick absorber layer are shown. In terms of the parasitic absorptions, the p-layer and the front zinc oxide layer absorb 8.5\% and 22\%, respectively, of the total absorbed light in the entire solar cell stack. In contrast, the absorption in the n-layer of silicon and in the zinc oxide layer in the back is very low, accounting for a loss of less than 2\% to 3\%. Since a perfect back reflector was assumed, the loss in the back contact is zero. It is to be noted that in the model used in this study, the substrate was assumed to be a non-absorbing glass. Therefore, in the case of a real solar cell, a large fraction of the parasitic p-layer absorption will actually be absorbed in the glass substrate (e.g., borosilicate glass has a very low transmission at \( \lambda < 350 \) nm). The absorption in the glass substrate will not affect the short circuit current calculated from the absorption in
Figure 7.11: Quantum efficiency of the i-layer silicon diode and parasitic absorptions in the silicon p-layer and front zinc oxide layer. The absorptions in the n-layer silicon and back zinc oxide are not shown because they are almost negligible. The Yablonovitch limit is shown with dashed lines. Cases with a silicon diode thickness of 0.5 $\mu$m and 2.5 $\mu$m for a pyramid texture period of 1200 nm and a height of 400 nm are shown in (a) and (b), respectively.
the i-layer silicon. The largest loss in the p-layer is observed for the shorter wavelengths (from 300 nm to 500 nm). The p-layer is almost transparent for longer wavelengths. The absorption loss in the front zinc oxide layer for shorter wavelengths accounts for almost 35% of the total absorption. In the wavelength range of 500 nm to 800 nm, the absorption in the front zinc oxide is minimized. For longer wavelengths, the optical loss in the aluminum doped front zinc oxide layer increases due to the free carrier absorption. As compared to the theoretical absorption limit, between wavelengths of 500 nm and 950 nm, more than 18% of the incident light is lost due to reflection. For such thin solar cells, the potential of minimizing the parasitic absorption is small as compared to the gain that can be achieved by reducing the reflection and guiding the light within the absorber layer. Therefore, a reduction of the reflection should be the key point in designing thin solar cells, where the absorber is significantly thinner than the absorption length for longer wavelengths. For such thin solar cells, the period and height of the pyramid have to be reduced so that the diffracted light can interfere with light from neighboring unit cells.

By increasing the thickness of the absorber layer to 2.5 \( \mu m \) [Fig. 7.11(b)], the reflection of the solar cell is greatly reduced as compared to the theoretical absorption limit. The quantum efficiency can be increased by reducing the parasitic absorption in the front zinc oxide and silicon p-layer, particularly for the longer wavelengths. The reflection losses in thicker solar cells are smaller than those of thinner solar cells; therefore, efficient light management that reduces reflection loses is more beneficial for solar cells with smaller absorber thicknesses.

### 7.3.1 Minimizing Losses in the Solar Cell

A better incoupling of the incident light into the silicon diode reduces the reflection and concurrently enhances the quantum efficiency. Solar cells deposited on textured glass or double textured TCO layers improve the incoupling of the incident light into the silicon cell. Cross sections of both these structures are shown in Fig. 7.12. Fig. 7.12(a) exhibits the cross section of a solar cell prepared on a textured glass substrate. After patterning the glass, a 500 nm TCO layer is conformally deposited on the patterned glass substrate. Through the patterning of the glass substrate, the average thickness of the TCO layer is reduced by \( h_g / 3 \), where \( h_g \) is the height of the pyramid texture. Reducing the average thickness of the zinc oxide layer leads to a drop of the lateral conductivity of the zinc oxide film. To compensate for the drop in the lateral conductivity, the thickness of the zinc oxide layer was increased by \( h_g / 3 \). Therefore, we can compare the relative change in the short circuit current between solar cells prepared on patterned glass substrates and the devices discussed in the preceding section. The FDTD simulation of the solar cell on a patterned glass substrate exhibits a gain of al-
Figure 7.12: Schematic of solar cells deposited on (a) a textured glass substrate and (b) a double textured TCO. Better incoupling of the incident light leads to additional improvement in the short circuit current.

most 0.2 mA/cm² for a 500 nm thick solar cell (a pyramid height of 400 nm and a period of 1200 nm) as compared to the textured solar cell (with a similar period and height) deposited on a smooth glass substrate [Fig. 7.8(a)]. The gain is reduced to 0.1 mA/cm² when the absorber layer thickness is increased to 2500 nm while keeping the other parameters of the texture constant. Patterning of the glass substrate can be achieved via laser texturing of the substrate, wet etching in hydrofluoric acid, a sandblasting process, or ion beam treatment [126, 127]. The highest efficiency reported for micromorph tandem solar cells has also been achieved through a combination of patterned glass and textured TCO front contact [8].

The incoupling of the incident light can also be enhanced by using a double texture as shown in the schematic in Fig. 7.12(b). The regular surface texture is covered with spikes of significantly smaller dimensions than the incoming wavelength, such that the blue light can be efficiently coupled into the absorber layer. The smaller spikes act as an effective refractive index matching layer for the shorter wavelengths. The larger surface texture diffracts the longer wavelength light. The double texture combines the advantages from both of the regimes as described in the previous section. In the
optical simulations, spikes with a base period of 70 nm × 70 nm was added on top of a regular pyramid texture with a width of 700 nm. Because the blue incoupling is independent of the thickness of the absorber layer, for both 500 nm and 2500 nm thick absorber layers, the blue incoupling of the light was improved by 0.15 mA/cm². Similar observations have also been reported in experimental results presented in the literature, where improvements of the spectral response were observed for the blue as well as the red part of the spectrum [60, 61].

Further improvements in the solar cell performance can be achieved by decreasing the absorption of the TCO layer. The optical properties of the TCO film can be controlled by varying the doping concentration of aluminum or gallium in the ZnO film. However, the doping concentration will have an influence on the optical bandgap (bandgap widening/Burstein Moss shift) and the free carrier absorption [47, 50, 51]. Furthermore, the series resistance of the solar cell is increased. Therefore, this possibility will not be discussed within the scope of this work.

In terms of the parasitic absorption, the absorption of light in the p-layer leads to additional optical losses of 1.93 mA/cm² and 1.43 mA/cm² for the 500 nm and 2500 nm thick solar cells. This absorption of light in the doped microcrystalline silicon layers can be reduced by using hot wire deposited silicon carbide layers. So far, the doping of hot wire deposited silicon carbide films has been demonstrated for microcrystalline silicon n-layers [128]. The hot wire deposited films exhibit a significantly increased optical bandgap. As a consequence, the absorption coefficient for shorter wavelengths is reduced by one order of magnitude. Chen and coworkers developed an n-side illuminated n-i-p solar cell that exhibited short circuit currents of up to 25.6 mA/cm² for a 1 µm thick solar cell [129]. The simulation results showed that the absorption in the p-layer of a 1 µm thick solar cell corresponds to a loss in the short circuit current of 1.60 mA/cm². Therefore, by lowering the absorption in the p-layer, the short circuit current in the silicon diode can be enhanced by more than 1 mA/cm².

Absorption losses or plasmonic effects in the back reflector were also not considered in the FDTD simulations. Depending on the design of the back contact, they might help to increase or decrease the absorption of light in the absorber layer.

7.3.2 Randomly Textured Versus Periodic Textures

From this study on square based pyramid textured solar cells, a maximum short circuit current of 22.5 mA/cm² was determined for a pyramid period of 1200 nm and a pyramid height of 500 nm. At this stage, it remains unclear whether this value of the simulated short circuit current represents an absolute maximum of the short circuit current. The optical simulations depend on the shape of the base of the pyramidal texture. Changes in the base will have an influence on the short circuit current. Further
investigations are needed in order to study the influence of the base of the pyramids on the short circuit current.

Experimental results show that the short circuit current of a solar cell with an absorber thickness of 1 \( \mu \)m prepared on a randomly textured substrate can be enhanced up to 23.4 mA/cm\(^2\) as compared to the 16.3 mA/cm\(^2\) achievable in a smooth solar cell [47]. A surface analysis of HCl textured zinc oxide substrate shows that 45% to 60% of the substrate’s surface is covered with features that have optimal dimensions for light trapping (with a period in the range of the incident longer wavelengths). A small fraction (1% to 5%) of the surface area is covered by structures smaller than the optimal surface texture. The dimension of the remaining 30% to 40% is covered by structures that are larger than the optimal surface texture. This means that even though the randomized surface texture leads to a distinct increase of the short circuit current, the gain of the short circuit is not optimal. An analysis of the experimentally measured quantum efficiency reveals that the front thickness of the zinc oxide layer and the p-layer is thinner than the thicknesses used in this simulation study. It can be expected that a periodic structure will provide a higher short circuit current than a random textured surface. Recent results for periodically patterned solar cells with very thin amorphous silicon absorber layers have already shown very promising results [130, 131]. However, the manufacturing of the randomly textured TCO is rather inexpensive as compared to the preparation of periodic structures over large areas.

### 7.4 Summary

In this chapter, the optical wave propagation in microcrystalline thin-film silicon solar cells with pyramidal surface textures was investigated and compared to theoretical light trapping limits. The influence of the texture period, texture height, and microcrystalline silicon diode thickness on the short circuit current and quantum efficiency was investigated. The short circuit current is maximized for pyramid periods ranging from 700 to 1200 nm and heights of 400 to 500 nm. A comparison of the simulated quantum efficiencies and short circuit currents with the theoretical light trapping limit shows that the structures approach the limits with increasing solar cell thickness. In order to improve the absorption in the silicon i-layer, the parasitic losses in the solar cell have to be minimized. In terms of the optical enhancement of the short circuit current, thinner solar cells exhibit the most relative gain. For a solar cell with an absorber thickness of 500 nm, the simulated solar cells exhibit a gain of 106%. This relative gain decreases to 27% for an absorber thickness of 3500 nm. The major loss mechanism for thin solar cells is reflection and not absorption losses. Efficient light trapping techniques that can guide the propagating light within the absorber become more crucial as the solar cells get thinner.
Chapter 8

Summary and Outlook

8.1 Summary

As we proceed towards the future with more cost efficient solar cells, the absorber layer of thin-film silicon solar cells are inversely getting thinner. Therefore the importance of efficiently absorbing the incident light within very thin absorber layers becomes more crucial. In order to design optically efficient solar cells, it is imperative to understand the interplay between the optical wave propagation within the cell and the surface texture at its interfaces. Within the scope of this thesis, the influence of periodic surface texture was investigated by rigorously solving the Maxwell’s equations in two- and three-dimensions. By studying the varying parameters in surface textured solar cells, their performance in terms of the quantum efficiency and short circuit current was evaluated. The results have given us valuable understanding of the underlying physics of optics in such textured solar cells and insights onto how such surface textures can be tuned to harvest the incident light more efficiently.

The study of surface textured solar cells began with the simplest of surface texture: one dimensional line gratings. Even though the line grating structure is far from the textured substrates used in reality, the results from this study gave us an understanding on the role of texture period and height on the optical properties of the solar cell. By independently looking at the influence of height and period of the front and back gratings, it was learned that the combination of the two phase gratings is what determines the cell’s overall optical property. The optical simulations from this work were verified by comparing them to experimentally prepared solar cells deposited on substrates with line grating. A good agreement between the simulated and experimentally measured short circuit current were found. Under red and infrared illumination (wavelength 600-1100 nm) the maximum of the short circuit current of 11.3 mA/cm² was observed for a grating period of 600 nm. The simulations results also show that for a given period, the short circuit current is maximized if the groove height is approximately equal...
to half of the grating period.

In the next chapter the solar cell texture was modified to include triangular texture at its interfaces. A larger domain of period of the surface texture was also swepted, where the optics changed from the domain of effective refractive index region to geometrical optics region. Due to better incoupling in the effective refractive index region, the solar cells with periods smaller than 200 nm showed improved response in the blue part of the spectrum (wavelength 300-500 nm). And enhanced red and infrared current (wavelength 700-1100 nm) was achieved when the triangular texture was in the range of the incident longer wavelengths. The solar cell with triangular texture showed enhanced absorption when the opening angle of the texture was equal or close to 90°.

Taking advantage of the fact that this study looked at periodic surface texture, the optical simulations were also performed using rigorous coupled wave analysis (RCWA). By making some simple assumptions, this method provided a much faster computation for the two-dimensional structures. Both the line grating and triangular texture were investigated and compared to the short circuit current of 13 mA/cm² for a solar cell on a smooth substrate, the short circuit current was increased by around 60% for the textured solar cells. The approach based on RCWA was further utilized to analyze line scans of randomly textured zinc-oxide substrates.

In the final chapter of the results, solar cells deposited on three-dimensional pyramids were simulated. Along with the period and height of the square based pyramids, the thickness of the absorber layer was also varied. Compared to the two-dimensional surface textured solar cells, the maximum short circuit current increased by almost 2 mA/cm² for pyramid textured solar cells. This enhancement occurs due to the additional diffraction plane arising from a three-dimensional texture. By adapting the Yablonovitch limit for the simulated model system, the maximum short circuit current of the solar cells was calculated from an optically optimized perspective. The calculated quantum efficiencies were compared with the maximum possible absorption in the solar cells and the dominant optical losses for thin (500 nm) and thick (2500 nm) solar cells were identified. As the solar cells gets thinner, reduction of reflection losses become more crucial where the incident light should ideally be traveling along the planes of the solar cell interfaces after being diffracted at the front or back grating structure. With regards to reducing parasitic absorption losses, the idea of utilizing textured glass substrate and double textured transparent conductive oxide layer were integrated into the solar cell. It was shown that these techniques reduce the parasitic losses in the front transparent conductive oxide and the absorberd energy from that layer can be transferred to the i-layer of the silicon diode.
8.2 Further Areas to Investigate

Within the scope of this thesis, the optical simulation results were concentrated on periodically textured thin-film silicon solar cells. But in reality, the surface texture in the solar cells are ordered randomly where the period and height of such textures can vary significantly (e.g. AFM images shown in Fig. 2.13 on page 25). The analysis of such textured surfaces can be done with AFM (Atomic Force Microscopy) which gives us the height profile and statistics on the surface, such as rms-roughness and height distribution \[132\]. Along with the height information, the spatial distribution with regards to the period is also a necessary quality which determines the light trapping potential of a surface. By looking at the PSD (power spectral density) of the AFM image, we can obtain information regarding its spatial distribution \[133, 134\]. In order to get a more accurate representation of the surface texture, a tuple of \(<\text{period}-\text{height}>\) information would be desirable. Such information can be obtained by running an image segmentation algorithm on the AFM image. In my research group at Jacobs University, we have developed such an approach which segments the individual craters from the surface image data. The algorithm first finds all local minima (crater tips) and then subsequently determines the corresponding surrounding borders. Examples of such segmentation on two commonly used substrate for thin-film silicon solar cells, namely Asahi-U substrate and zinc-oxide substrate etched in dilute HCl, are shown in Figs. 8.1(a) and 8.1(d). The borders of the individual craters are marked by black lines, while the minima (tips) of the craters are marked by white points. The surface of the two textured films were approximated as an arrangement of pyramids (Asahi-U) and craters (textured zinc-oxide). In such an arrangement the dimensions of the pyramids or craters can be described by the diameter and depth of the features. The distributions of the diameters and depths of the two substrates are also shown in Fig. 8.1. Figs. 8.1(b) and 8.1(c) correspond to the distribution from the Asahi-U substrate. It can be observed that the peak of the diameter distribution occurs in between 300 - 400 nm. The distribution of the depth peaks at heights around 80 - 90 nm. Contrary to what is observed for the distribution of Asahi-U substrates, the distribution of the diameter from zinc-oxide substrate etched in dilute HCl is much broader with dimensions ranging from 200 nm up to 2000 nm. In terms of the depth of the craters, textured zinc-oxide substrate also contain much deeper features with depth of more than 500 nm.

A detailed description of this method is beyond the scope of this thesis, but interested readers can find more about the segmentation method in Ref. \[135\]. Previous work from Haase \textit{et al.} has already shown that contributions from individual craters superimpose to form the response from the entire textured substrate (Haase and coworkers did their studies for periodic and quasi-random structures) \[122\]. Thus
Figure 8.1: Surface segmentation of (a) Asahi-U substrate and (d) ZnO substrate etched with dilute HCl. Pyramid/crater diameter and depth distributions for Asahi-U substrates are shown in (b) and (c) and the distributions for HCl textured ZnO substrates are shown in (e) and (f). Substrate area of the images are 10 µm x 10 µm.
8.2. Further Areas to Investigate

in tandem to the simulation results from this work, surface segmentation data would provide a stronger prediction tool for the optical response from textured substrates. I would like to refer back to the short circuit current map depicted in Fig. 7.3 on page 93 of chapter 7. In Fig. 8.2, the exact short circuit current map is reproduced in gray-scale color with the distribution tuple of <period-height> for Asahi-U substrate and textured zinc-oxide substrate overlaid on top of the plot. The dense blue markers represent the distribution of Asahi-U substrates and the distribution of textured zinc-oxide substrate is shown with red markers. Intuitively just by looking at the figure, one gets a feeling that for a 1 \( \mu \text{m} \) thick microcrystalline silicon solar cell, the performance of solar cells on a textured zinc-oxide substrate should be higher than the cell deposited on Asahi-U substrates. This intuitive feeling about the performance of the solar cell can of course be quantified and calculated. Thus, further work on connecting the optical simulation results with the surface distribution data needs to be done.

Another domain which has been assumed to ideal in this study was the back contact of the solar cell. From experimental results, it is well known that the back contact contributes a lot towards the optical losses in a solar cell as well [136, 137]. In Fig. 8.3 the quantum efficiencies and the optical losses in all the other layers of the solar cell are shown for solar cells with a perfect metal as a back contact and with silver as the back contact. Both the solar cells consisted of a 1 \( \mu \text{m} \) thick absorber layer with a
pyramid texture of period 500 nm and height of 400 nm. In Fig. 8.3(a) where a perfect metal with 100% reflectivity was used as the back contact, the absorption losses in the n-layer silicon and back zinc-oxide are almost negligible. These parasitic contributions are therefore not shown in the figure. By changing the back contact to silver in Fig. 8.3(b), increase in the parasitic losses at the back contact of the solar cell is observed. The losses increase for wavelengths of the incident light longer than 450 nm. Due to plasmonic effects, the absorption losses in the back zinc-oxide layer, which is in contact with the silver layer, is greatly enhanced. Since the absorption losses increase, a decrease in the quantum efficiency after introducing the silver back contact is also observed. Compared to the 21.40 mA/cm$^2$ achieved for the solar cell with perfect metal back contact, a decrease of 21% resulting into short circuit current of 17 mA/cm$^2$ is obtained for the same solar cell with silver back contact. The choice on the type of the metal as a contact, along with the combination of ZnO-metal, also proposes some open questions with regards to the optics. In recent years, the use of white paint as a highly reflective back contact has also gained considerable interest [138, 139]. Moreover, the use of metal nanoparticles to act as plasmon scatterers has also accelerated the field of investigating plasmonic solar cells [140–142]. Experimentally such scatterers have been deposited at the front [143, 144], back [145] and also inside [146] of the solar cell. By utilizing metallic nanoparticles enhanced absorptions has been reported for ultra-thin silicon solar cells [147, 148]. The optical results from this study can therefore be further complemented by investigation of the back contact of the solar cell.

Optical simulations of silicon solar cells deposited on randomly textured substrates has also been recently reported [149, 150]. But understanding the physics of optics in such a device is not trivial. Simpler assumptions with regards to the structure of the solar cell have to be made in order to understand the optical propagation in such a device. Investigation of the optical response at the textured surfaces using near-field scanning optical microscopy (SNOM) can be beneficial in understanding the near-field optics in such randomly textured substrates [151]. Or by tuning the randomness of the surface with a scaling factor can also lead to better understanding on the optics of such surfaces [152, 153]. While the transition from periodically to randomly textured substrates might not be just a one step process, but it is a research idea that has be kept in the bigger picture. Nevertheless, the results from this study provide a solid foundation in exploring into more intricate issues which are intertwined with the optical response of thin-film silicon solar cells. With optics playing a major role in enhancing the absorption efficiencies of thin-film silicon solar cells, there still awaits exciting areas of research which are yet to be solved.
Figure 8.3: Quantum efficiency of the i-layer silicon diode and the parasitic absorption losses in all the other layers of 1 um thick microcrystalline silicon solar cells with pyramid texture of period 500 nm and height of 400 nm. In (a) the back contact was modeled using a perfect metal with 100% reflectivity. Thus the absorption losses in the n-layer silicon and back zinc-oxide are almost negligible and therefore not shown. By introducing silver (Ag) as the back contact in (b), parasitic absorptions in the metal contact, back zinc-oxide and n-layer silicon are greatly enhanced.
Bibliography


# List of Symbols and Acronyms

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
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<tbody>
<tr>
<td>$\alpha$</td>
<td>Attenuation or absorption coefficient $[m^{-1}]$</td>
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<tr>
<td>$\epsilon$</td>
<td>Electrical permittivity. (In free space $\epsilon_0 = 8.854 \times 10^{-12} \text{ F/m}$)</td>
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<tr>
<td>$\eta$</td>
<td>Conversion efficiency of a solar cell</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>Wavelength of the incident light $[m]$</td>
</tr>
<tr>
<td>$\mu$</td>
<td>Magnetic permeability. (In free space $\mu_0 = 4\pi \times 10^{-7} \text{ H/m}$)</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Electrical charge density $[\text{C/m}^3]$</td>
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<tr>
<td>$\sigma_{\text{rms}}$</td>
<td>Root mean square roughness $[m]$</td>
</tr>
<tr>
<td>$\tilde{n} = n + ik$</td>
<td>Complex refractive index</td>
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<tr>
<td>$c$</td>
<td>Speed of light. (In free space $c_0 = 3 \times 10^8 \text{ m/s}$)</td>
</tr>
<tr>
<td>$E_g$</td>
<td>Bandgap of a material $[\text{eV}]$</td>
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<tr>
<td>$h$</td>
<td>Planck’s constant. $(6.626 \times 10^{-34} \text{ Js})$</td>
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<tr>
<td>$k$</td>
<td>Boltzmann’s constant. $(1.38 \times 10^{-23} \text{ J/K})$</td>
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<tr>
<td>$q$</td>
<td>Elementary charge. $(1.602 \times 10^{-19} \text{ C})$</td>
</tr>
<tr>
<td>$B$</td>
<td>Magnetic flux density $[\text{Wb/m}^2]$</td>
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<tr>
<td>$D$</td>
<td>Electric flux density $[\text{C/m}^2]$</td>
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<tr>
<td>$E$</td>
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<td>$J$</td>
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<td>$\mu\text{c-Si:H}$</td>
<td>Hydrogenated microcrystalline silicon</td>
</tr>
<tr>
<td>$\text{a-Si:H}$</td>
<td>Hydrogenated amorphous silicon</td>
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<tr>
<td>AFM</td>
<td>Atomic force microscopy</td>
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<tr>
<td>Acronym</td>
<td>Description</td>
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<tr>
<td>Ag</td>
<td>Silver</td>
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<td>AM 1.5</td>
<td>Reference solar spectral irradiance. Air Mass 1.5</td>
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<td>APCVD</td>
<td>Atmospheric pressure chemical vapor deposition</td>
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<td>C-method</td>
<td>Chandezon method</td>
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<td>c-Si</td>
<td>Crystalline silicon</td>
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<td>CdTe</td>
<td>Cadmium telluride</td>
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<td>CIS/CIGS</td>
<td>Copper indium (gallium) deselenide</td>
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<td>EMT</td>
<td>Effective medium theory</td>
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<td>FDM</td>
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<td>Finite integration technique</td>
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<td>HCl</td>
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<td>Modal method</td>
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<td>MoM</td>
<td>Method of moments</td>
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<td>PSD</td>
<td>Power spectral density</td>
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<tr>
<td>RCWA</td>
<td>Rigorous coupled wave analysis</td>
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<tr>
<td>SEM</td>
<td>Scanning electron microscopy</td>
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<tr>
<td>SNOM</td>
<td>Near-field scanning optical microscopy</td>
</tr>
<tr>
<td>TCO</td>
<td>Transparent conductive oxide</td>
</tr>
<tr>
<td>TE</td>
<td>Transverse electric polarized light</td>
</tr>
<tr>
<td>TM</td>
<td>Transverse magnetic polarized light</td>
</tr>
<tr>
<td>ZnO:Al</td>
<td>Aluminum doped zinc oxide</td>
</tr>
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</table>
Publications and Conference Presentations

Parts of this thesis have already been published or presented elsewhere.

Publications Related to this Thesis


Other Publications


Conference Presentations


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• I would like to acknowledge my supervisor, Prof. Dr. Dietmar Knipp, for providing me the opportunity to work in this exciting project. His continued encouragement and support has been pivotal in the completion of this thesis project. He has shown me how to do research and how to think like a researcher. Most of what I know about solar cells, optics and device physics has been an accumulation from myriad of discussions I had with Prof. Knipp in lectures, group meetings, coffee meetings or mostly my spontaneously dropping by his office with a question in my mind. I thank him for sharing his knowledge with me.

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