Characterization and modeling of nanostructured silicon thin-film optoelectronic devices

by

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Declaration

I, Vladislav Jovanov, hereby declare that I have written this PhD thesis independently, unless where clearly stated otherwise. I have used only the sources, the data and the support that I have clearly mentioned. This PhD thesis has not been submitted for conferral of degree elsewhere.

Bremen, 09.04.2015.

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Signature
Abstract

Design and fabrication at nanometer scale level have enabled development of novel optoelectronic devices. These devices take advantage of the optical phenomena that occur when light interacts with structures that are smaller than the wavelength of the incoming light. Depending on how these structures are employed, different functions can be achieved. When the thickness of devices is a fraction of the wavelength, they become transparent. On the other hand, optoelectronic devices become highly absorbing, when nanostructures are introduced at their interfaces. In this research, silicon thin-film optoelectronic devices with nanostructured layers and interfaces are studied.

An ultra thin-film transparent photodetector is used to experimentally realize standing wave and transparent Fabry-Perot spectrometer. Optical models for these devices are developed using an analytical approach to solve Maxwell’s equations. Excellent agreement between experimental and calculated results is demonstrated. The linear setup of these spectrometers, allows for the realization of spectral imaging cameras where the spectrum of the light source is obtained by the Fourier transform of the detector signal.

The performances of silicon thin-film solar cells deposited on randomly textured substrates are investigated experimentally and by optical simulations. The investigation has been focused on the back contact losses. A comparison of experimental results and optical simulations reveals that the back contact losses are influenced by plasmonic resonances only when the nanofeatures are present at the interface between a metal reflector and solar cell. The plasmonic losses can be reduced by introducing a transparent conductive oxide buffer layer or by removing the nanofeatures. The optimization of the back contact leads to improved performances of silicon thin-film solar cells.
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Part I

Introduction
Chapter 1

Introduction

1.1 Motivation

The development of novel optoelectronic devices requires design and fabrication at nanometer scale level [1, 2]. In optoelectronic devices, every structure that is smaller than the wavelength of the incoming light can be considered as a nanostructure. To realize optoelectronic devices with novel properties and functions, one should take advantage of optical phenomena that occur when light interacts with the nanostructures. In recent years, the high demand for novel optoelectronic devices has been seen in areas such as spectral imaging and photovoltaic. In the following, the motivations for these two areas are presented.

1.1.1 Spectral imaging

Spectral imaging is crucial for fields such as high performance color acquisition and reproduction [3, 4], remote-sensing and target detection [5, 6], medical-imaging for pigment recognition and skin cancer detection [7, 8], and food quality control [9]. Spectral imaging is developed to fill the gap between standard imaging and spectrometry. Standard image systems provide information about objects with high spatial, but relatively low spectral resolution consisting only of three color channels. On the other hand, laboratory spectrometers exhibit high spectral resolution without any spatial information. Spectral imaging systems combine spatial resolution of a standard imaging system with spectral resolution of a spectrometer. Consequently, a spectral image of an object is a three dimensional (3D) data set consisting of two spatial and one spectral dimension.

Spectral imaging applications require compact and portable devices with low manufacturing costs and good performance. To develop spectral imaging systems, spectrometers such as grating and Michelson have been miniaturized [10–13]. The advantage of Michelson spectrometer is its ability to collect spectral information for all wavelengths during a single scan, which is a common feature for all spectrometers that fall into a class of Fourier transform spectrometers [14, 15]. However, to create spectral imaging systems it is necessary to realize two dimensional (2D) spectrometer arrays. Michelson spectrometers exhibit 2D geometry, which does not allow for dense integration on a single chip [12, 13]. To overcome this problem, spectrometers with linear setup based on the sampling of a standing wave have been proposed [16].

Sampling of a standing wave requires transparent photodetectors with nanometer
thickness. In recent years, advances in nanotechnology have led to the development of transparent photodetectors and standing wave spectrometers [17–20]. To form a standing wave spectrometer, a transparent photodetector has to be placed in front of a mirror. The realization of spectral imaging systems is easily achieved by dense integration of 2D arrays of transparent photodetectors on a single chip. Furthermore, transparent photodetectors can also be used for the development of Fabry-Perot spectrometers that operate in transmission [21]. To fully understand advantages and disadvantages of these optoelectronic devices, a precise characterization and modeling is required.

1.1.2 Photovoltaic solar cells

Increasing demand for energy from renewable sources has lead to development of photovoltaic industry. Since sunlight is freely available, photovoltaic industry has the potential to become a primary source of renewable energy. Currently, more than 80 % of the photovoltaic market is being held by crystalline silicon (c-Si) wafer based solar cells [22]. The success of the c-Si solar cells is influenced by well established microelectronic production technologies and their high energy conversion efficiencies of almost 25 % [23]. The thickness of c-Si solar cells is around 180 µm, since c-Si wafers are produced by mechanical cutting of ingots.

To reduce the material usage and fabrication costs, researches have turned to the thin-film technology. With this approach thin layers of silicon materials are deposited on a low cost substrates such as glass or flexible plastic [24, 25]. Furthermore, thin-film deposition techniques are compatible with large area substrates which allows for mass scale production. Despite these advantages, thin-film solar cells are still unable to substitute the c-Si solar cells on the market due to their low conversion efficiencies. Single junction thin-film solar cells with organic materials as absorber can exhibit conversion efficiencies up to 10 % [26, 27]. On the other hand, silicon thin-film solar cells can exhibit conversion efficiencies of more than 10 % depending on the material system and configuration [28–33]. To gain larger piece of the photovoltaic market, thin-film solar cells have to be improved by reducing production costs and increasing conversion efficiencies.

Conversion efficiencies of silicon thin-film solar cells can be enhanced by introducing light trapping schemes or reducing the optical losses. To identify sources of optical losses, solar cells have to be accurately modeled and analyzed. By gaining deeper understanding of light propagation within the solar cells, optical losses can be minimized, and conversion efficiencies can be increased.

1.2 Thesis outline

In this thesis, different types of optoelectronic devices are investigated. Therefore, the main results are divided into two parts. Part II deals with the optoelectronic devices with nanostructured layers, which are represented by transparent photodetector and its spectrometer applications. The optoelectronic devices with nanostructured interfaces, which are represented by silicon thin-film solar cells deposited on randomly textured substrates, are focus of Part III.

To model optoelectronic devices, it is necessary to solve Maxwell’s equation, and determine the light propagation within a device. Therefore, basics of electromagnetic
are introduced in Chapter 2. Furthermore, this chapter gives an overview of materials and processes used for the fabrication of optoelectronic devices that are in the focus of this thesis. Since transparent photodetectors and its spectrometer applications exhibit simple geometry, Maxwell's equations are solved using analytical approaches. By using the analytical approach, performances of the transparent photodetector such as quantum efficiency and transmission are modeled.

Chapter 3 focuses on spectrometer applications of the transparent photodetector. Different types of spectrometers have been experimentally realized and accurately modeled. Based on the optical models, the operating range of standing wave and Fabry-Perot spectrometers are precisely determined. Furthermore, optical models for partially coherent light are also developed and presented.

The fundamentals of solar cells are explained in Chapter 4. This chapter is focused on silicon thin-film solar cells. Different ways to introduce light trapping are presented and analyzed using image segmentation algorithm. For the first time, a simple geometrical tool is developed, which can accurately predict the silicon film formation on a textured surface. Furthermore, an overview of numerical approaches to solve Maxwell’s equations is given. The numerical approach is compared to analytical modes for silicon thin-film solar cells without textured interfaces.

Chapter 5 investigates the back contact losses in silicon thin-film solar cells. Accurate optical models are used to describe the experimental data and provide deeper understanding of light absorption in metal back reflectors. For the first time, the plasmonic and non-plasmonic back contact losses are identified. Finally, design rules to minimize back contact losses are presented.

In the end, Chapter 6 presents future areas of investigation of optoelectronic devices with nanostructured layer and interfaces. An approach how to improve performances of spectrometers based on transparent photodetectors is presented and discussed. Furthermore, different ways to improve the optical models of silicon thin-film solar cells are shown and compared.
1. Introduction
Part II

Optoelectronic devices with nano-structured layers
Chapter 2

Transparent photodetector

The development of transparent photodetectors has been initiated by the increased interest for realization of miniaturized spectrometer and interferometer systems based on the sampling of a standing wave [16]. Several types of transparent photodetectors with different materials and designs have been realized in the past two decades [17–19, 34–37]. The main requirements that transparent photodetectors have to fulfill are high transmission and sufficient photosensitivity.

To achieve operation in transmission, the photodetector has to be ultra thin. On the other hand, to generate a detectable electrical signal, the thickness of the photodetector cannot be reduced below certain value. Due to this trade-off, special considerations have to be given to the design of the transparent photodetector.

The goal of this chapter is to provide some insights into the design and fabrication of the transparent photodetector that is used to realize standing wave and Fabry-Perot spectrometers. Furthermore, different optical models that are able to determine the light propagation through optically thin or thick multilayer systems are presented. In the end, the quantum efficiency and transmission of the transparent photodetector are calculated using developed optical models and compared to the measured data.

2.1 Photodetectors - fundamental concepts

Photodetectors are optoelectronic devices developed to sense light and generate an electrical signal. Depending on the detection process, photodetectors can be classified as thermal or photon detectors.

Thermal detectors detect the temperature change on their surface when exposed to light. Thermal detectors such as microbolometers exhibit change of the resistivity with temperature, which is used to detect far-infrared wavelengths.

Photon detectors are based on the quantum photoelectric effect, where photons are directly absorbed. Absorption of a photon excites an electron and creates electron-hole pair, which contributes to the photocurrent (photoconductors, photodiodes) or accumulated charges (charge - coupled devices (CCD) image sensors).

 Majority of the optical photodetectors in the commercial market are photon detectors where a semiconductor is used as the active material. For light to be absorbed, the photon energy has to be larger than the band gap of the semiconductor. The maximum wavelength that can be absorbed by the photodetector ($\lambda_{max}$) is defined
2. Transparent photodetector

by:

\[ \lambda_{\text{max}} = \frac{h \cdot c}{E_g} \]  

(2.1)

where \( c \) is the speed of light, \( h \) is Planck’s constant, and \( E_g \) is the energy gap of the semiconductor [38]. Depending on the semiconductor material and the detector type, the operating range of photodetectors can be tuned to cover specific regions of the optical spectrum.

The light absorption in the photodetector is determined by the optical constants of the semiconductor. The optical constants are described by the complex refractive index:

\[ N = \eta - i \cdot \kappa \]  

(2.2)

where \( \eta \) is the refractive index of the material, and \( \kappa \) is the extinction coefficient. The extinction coefficient defines the absorption coefficient (\( \alpha \)) of the material:

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

(2.3)

where \( \lambda \) is the wavelength of the incoming light. A high value of the absorption coefficient means that the light will be absorbed near the surface of the semiconductor. On the other hand, a low value of the absorption coefficient indicates that the light penetrates deep into the semiconductor before it gets absorbed. If the thickness of the semiconductor is sufficiently small, a certain amount of light is able to pass through without being absorbed, and the photodetector becomes partially transparent.

The absorption properties of the semiconductor material determine the sensitivity of the photodetector. The basic metric that defines the sensitivity of the photodetector is the quantum efficiency. The quantum efficiency (\( \text{QE} \)) represents the number of generated charge carriers per incident photon [38]:

\[ \text{QE} = \frac{|I_{ph}|}{q \cdot \Phi} = \frac{|I_{ph}|}{q} \cdot \frac{h \cdot \nu}{P_{in}} \]  

(2.4)

where \( I_{ph} \) is the photocurrent for the specific frequency of the light (\( \nu = c/\lambda \)), \( \Phi \) is the photon flux, \( q \) is the elementary charge, and \( P_{in} \) is the input optical power. The maximum value of the quantum efficiency is unity. However, due to optical and electrical losses, the value of the quantum efficiency is lower than one. The responsivity (\( \mathcal{R} \)) is also used to quantify the sensitivity of the photodetector. The responsivity represents the ratio between the generated photocurrent and optical power [38]:

\[ \mathcal{R} = \frac{|I_{ph}|}{P_{in}} \]  

(2.5)

High sensitivity of the photodetectors is necessary to generate a detectable electrical signal. Some photodetectors such as photoconductors and avalanche photodiodes have an internal current-gain mechanism, which amplifies the photocurrent. Other important requirements that photodetectors have to satisfy are high response speed and low noise.

Typical examples of optical photodetectors are: complementary metal - oxide - semiconductor (CMOS) image sensors, CCD, phototransistors, photoconductors, photodiodes, etc. A large variety of optical photodetectors is necessary to satisfy specific requirements for different applications. The applications of standard optical photodetectors range from imaging cameras to optical communication and measurement systems.
2.2 Development of transparent photodetectors

Transparent photodetectors are optoelectronic devices designed to detect light while operating in transmission. Therefore, figures of merit and requirements presented in Sec. 2.1 are also applicable in this case. To fully characterize transparent photodetectors, the transmission properties are also necessary. The transmission ($T$) is defined by:

$$T = \frac{P_{\text{out}}}{P_{\text{in}}}$$

(2.6)

where $P_{\text{out}}$ is the optical power that exits the transparent photodetector.

In the past two decades, several types of transparent photodetectors have been developed [17–19, 34–37]. Sasaki et al. realized transparent photodetector based on a p-n photodiode [17]. The transparent p-n photodiode has been fabricated in a coplanar configuration on a quartz substrate with c-Si as an active material.

More recently, Kung et al. developed a transparent photoconductor deposited in a coplanar configuration on a quartz substrate [18, 34]. Due to its internal current gain mechanism, the transparent photoconductor exhibits higher sensitivity than the transparent p-n photodiode. As active materials, amorphous silicon (a-Si) [34] and polycrystalline silicon (pc-Si) [18] have been used.

Photodetectors in a coplanar configuration exhibit a photocurrent flow normal to the incident light. The distance that generated charge carriers have to travel before they are collected is determined by the electrode spacing. The electrode spacing and material properties of the active material dictate the maximum operating speed of coplanar photodetectors [34]. For the realized transparent coplanar photodetectors, electrode spacing is minimized by using comb pattern of electrodes with distance between fingers of 30-40 $\mu$m [17, 34]. The transmission properties of coplanar transparent photodetectors depend on the thickness of the active layer and optical properties of materials [17].

By changing the photodetector configuration from coplanar to orthogonal, the operating speed and transmission properties can be improved. In orthogonal configuration, the photodetector is sandwiched between electrodes, and the flow of the photocurrent is parallel to the incident light. Therefore, the distance that generated charge carriers have to travel is defined by the thickness of the active layer. This thickness is in order of few dozens of nanometers [17–19, 34–36], and higher operating speeds can be achieved compared to coplanar photodetectors. In orthogonal configuration, electrodes have to be transparent so that the light can pass through. Transparent electrodes can be used as antireflection coatings to tune transmission properties of the transparent photodetector.

Stiebig et al. developed transparent photodetectors in orthogonal configuration based on a p-i-n photodiode using a transparent conductive oxide (TCO) to form the electrodes [19, 35]. Furthermore, Stiebig et al. realized a transparent photodetector with two p-i-n photodiodes and a phase shifter for directional interferometric measurements [36]. By changing the active material to gallium arsenide (GaAs), Bhalotra et al. realized transparent p-i-n photodiode in the near infrared region of the optical spectrum [37].

In this research, the transparent p-i-n photodiode developed by Stiebig et al. is used for experimental realization of standing wave spectrometer and Fabry-Perot spectrometer.
2. Transparent photodetector

2.2.1 Photodiodes

**p-n photodiodes.** Photodiodes are standard diodes designed to be exposed to light. In the diode junction between p- and n- type of the semiconductor, a space charge (depletion) region is formed. This region exhibits fixed charges (ionized dopants) and built-in electric field. When the photodiode is exposed to light, electron-hole pairs generated within depletion region are separated by the built-in electric field and do not recombine. The charge carriers generated outside depletion region have to diffuse to the junction.

Another important parameter of the photodiode is the operating speed. The operating speed depends on the transit time of charge carriers through the depletion region, capacitance of the depletion region and diffusion of charge carriers outside of the depletion region [38]. If the depletion region is thin, the transit time will be short, but at the same time the diode capacitance will increase. A wider depletion region exhibits lower capacitance but longer transit time. To optimize the depletion region width, a trade-off between the quantum efficiency and operating speed has to be taken into account.

The width of the depletion region is defined by the concentration of donors in the n-region and acceptors in the p-region of the diode. The depletion region is wider if the difference between concentrations is larger. By applying an external voltage to the photodiode, the width of the depletion region can be controlled. The reverse-bias voltage increases the width of the depletion region and the built-in electric field. Higher built-in electric field improves separation of generated electron-hole pairs and decreases transit time. At the same time, larger width of the depletion region results in higher quantum efficiency and lower photodiode capacitance. However, reverse biasing voltages have to be moderated or diode breakdown may occur.

**p-i-n photodiodes.** A different approach to control the width of the depletion region is by introducing a layer of an intrinsic semiconductor between the p- and n-region, which forms a p-i-n photodiode. In this case, the i-layer is totally depleted, and its thickness represents the width of the depletion region. Therefore, the concentration of dopants in both the p- and n-region can be high without any significant influence on the depletion region width [39]. This type of photodiodes can achieve high operating speeds and sensitivities [38, 39].

A schematic representation of a p-i-n photodiode, its energy band diagram, built-in electric field profile and light absorption profile are shown in Fig. 2.1. Typically, p-i-n photodiodes operate under reverse bias conditions [38, 39], which is shown in Fig. 2.1a. The reverse bias voltage ($V_R$) influences the energy band diagram (Fig. 2.1b) and strength of the built-in electric field (Fig. 2.1c). An energy band diagram of p-i-n photodiode is depicted in Fig. 2.1b. Figure 2.1b also shows absorption of photons within the i-layer and generation of electron-hole pairs. An internal electric field separates generated charge carriers by driving the electrons to the n-layer and holes to the p-layer. The profile of the built-in electric field is shown in Fig. 2.1c. Fixed ionized impurities in the p- and n-layer build up the electric field, which extends through the i-layer. Since the density of impurities in the i-layer is much smaller compared to the p- and n-layer, extensions of the depletion region within p- and n-layer are negligible compared to the i-layer thickness [39]. When the active material does not exhibit defects, the built-in electric field is constant across the i-layer (dash-doted line in Fig. 2.1c). For a reverse bias voltage that is significantly larger than the
2.2 Development of transparent photodetectors

\[ P_{in} \rightarrow \nabla \nabla R \cdot P_{in} \]

\[ E_C \quad \text{electrons} \]

\[ F \cdot \nu \quad \text{holes} \]

\[ E_F \]

\[ \sim \exp(-\alpha \cdot z) \]

\[ z_p \quad d_i \quad z_n \]

Figure 2.1: (a) Cross-section of a p-i-n photodiode. (b) Energy band gap diagram and charge separation under operating conditions. (c) Profile of the built-in electric field. (d) Power loss profile within p-i-n photodiode.

built-in potential \((V_R \gg \psi_{bi})\), the intensity of the electric field within the i-layer can be approximated by:

\[ E = \frac{V_R}{d_i} \tag{2.7} \]

where \(d_i\) is the thickness of the i-layer (width of the depleted region). The built-in electric field has to be large enough so that generated charge carriers drift across the i-layer at their saturation velocities [38]. In practice, the electric field within the i-layer is not uniform (solid line in Fig. 2.1c) due to the defects within the i-layer and its interfaces [40]. These defects originate from unintentional doping of the i-layer (ionized impurities) and trapped states (trapped charges). The electric field deformation depends upon material used for the i-layer and the thickness of the i-layer [40]. This is mainly important in solar cell applications, where p-i-n photodiodes are not reverse biased.

The photocurrent and quantum efficiency of p-i-n photodiodes can be calculated from a time averaged power loss profile. Figure 2.1d depicts the power loss profile within a p-i-n photodiode assuming that the light gets absorbed in one pass, and that the optical properties of the p-, i- and n-layer are equal. The time averaged power loss \((Q(z))\) profile is given by:

\[ Q(z) = \alpha \cdot I(z) \tag{2.8} \]
where \( I(z) \) is the light intensity (irradiance), and \( z \) represents a position within the p-i-n photodiode. The light intensity as a function of the position \( (I(z)) \) can be obtained from Beer-Lambert-Bouguer law. Beer-Lambert-Bouguer law relates light absorption to the properties of the material through which light is passing:

\[
\alpha = -\frac{dI(z)}{I(z)dz} \tag{2.9}
\]

Taking into account the boundary condition \( (I(0) = P_{in} \cdot (1 - R)/A) \), the solution of Eq. (2.9) is given by:

\[
I(z) = \frac{P_{in} \cdot (1 - R)}{A} \cdot \exp(-\alpha \cdot z) \tag{2.10}
\]

where \( R \) is the reflectivity of the p-i-n photodiode, and \( A \) is the device area. In general, the photocurrent is composed of a drift current (charge carriers generated within the i-layer) and diffusion current (charge carriers generated in the p- and n-layer) [38]. However, throughout this thesis, the following assumptions are used when calculating the photocurrent and quantum efficiency:

- thermal generation of charge carriers is neglected resulting in a zero dark current,
- charge carriers generated in the p- and n-layer recombine, and do not contribute to the photocurrent,
- only charge carriers generated in the i-layer contribute to the overall photocurrent, and
- all generated charge carriers are collected resulting in the internal quantum efficiency of one.

Under these assumptions the photocurrent \( (I_{ph}) \) of the p-i-n photodiode for a specific frequency/wavelength is given by [38]:

\[
I_{ph} = -\frac{q \cdot A}{h \cdot \nu} \int_{0}^{d_i} Q(z')dz' \tag{2.11}
\]

where \( z' = z - z_p \) represents a position within the i-layer. By replacing Eq. (2.10) into Eq. (2.8), and solving the integral in Eq. (2.11), the expression for the photocurrent is obtained:

\[
I_{ph} = -\frac{q}{h \cdot \nu} \cdot P_{in} \cdot (1 - R) \cdot \exp(-\alpha \cdot z_p) \cdot (1 - \exp(-\alpha \cdot d_i)) \tag{2.12}
\]

The quantum efficiency of the p-i-n photodiode is obtained by combining Eqs. (2.4) and (2.12), and it is given by:

\[
QE = (1 - R) \cdot (1 - A_p) \cdot (1 - \exp(-\alpha \cdot d_i)) \tag{2.13}
\]

where \( A_p \) represents the absorption of the p-layer \( (A_p = 1 - \exp(-\alpha \cdot z_p)) \). Qualitatively, the quantum efficiency of the p-i-n photodiode depends on the reflection losses of the diode surface, absorption losses in the front contact (p-layer for this analysis) and the absorption properties of the active layer.
2.2 Development of transparent photodetectors

2.2.2 Material properties

The operating range of photodetectors depends on the optical properties of the semiconductor material. Developed transparent photodetectors are mainly based on silicon materials [17–19, 34–36]. The energy band gap of silicon materials range from 1.7 eV for a-Si to 1.1 eV for microcrystalline silicon (µc-Si) and c-Si. According to Eq. (2.1), maximum wavelengths that can be detected are 730 nm for a-Si and 1130 nm for µc-Si and c-Si, respectively. Consequently, the operating range of fabricated transparent photodetectors completely covers the visible region of the electromagnetic spectrum.

To show the absorption properties of the hydrogenated amorphous silicon (a-Si:H), hydrogenated microcrystalline silicon (µc-Si:H) and c-Si materials, their absorption coefficients are adapted from literature [41–43].

The absorption coefficients of a-Si:H, µc-Si:H and c-Si are depicted in Fig. 2.2a. The absorption coefficient of a-Si:H is larger than that of µc-Si:H and c-Si for photon energies larger than its band gap. For photon energies smaller than the band gap the absorption coefficient of the a-Si:H drops significantly. Amorphous materials exhibit disorder in arrangement of atoms, and potential varies from position to position. Therefore, the boundaries of the valence and conductive band are blurry. If the disorder is large, the densities of states for the valence and conductive band exhibit tails, which extend into the energy gap [44]. These tail states allow for light absorption even if photon energies are smaller than the band gap. Consequently, the absorption coefficient of the a-Si:H is still larger than zero in this region. Electron-hole pairs generated due to the sub-bandgap absorption contribute to the photocurrent only if charge carriers end up in the conductive (electrons) or valence (holes) band. Therefore, electrical losses in this region are high, and it can be assumed that a-Si:H is non-absorbing for wavelengths larger than 800 nm. The absorption properties of the µc-Si:H are comparable to the c-Si for wavelengths longer than 850 nm (Fig. 2.2a). For shorter wavelengths, the absorption coefficient of the µc-Si:H is larger than for c-Si.

The operating range of photodetectors with a-Si:H as the active material is limited to the visible region of electromagnetic spectrum (300-800 nm). On the other hand, the operating range of photodetectors with µc-Si:H or c-Si as the active material is larger and covers the visible and near infrared region of the spectrum (300-1100 nm). For the visible region of the spectrum, a high sensitivity photodetector can be achieved by using a-Si:H due to its absorption properties.

To create transparent electrodes for optoelectronic devices, TCOs are typically used. TCOs are wide band gap oxide semiconductors with good electrical and optical properties, which are achieved by doping. In general, the optical properties of TCOs are influenced by the energy band gap and by free carrier absorption. For shorter wavelengths, TCOs act as typical semiconductors, and light gets absorbed directly since the photon energy is higher than the band gap. For longer wavelengths, TCOs show metal like behavior. The concentration of free charge carriers in the TCO is high, and they behave like electron gas in a metal. The plasma frequency/wavelength of the electron gas determines the light absorption. Close to the plasma wavelength, light is absorbed due to the free carrier absorption. If the light wavelength is lower than the plasma wavelength, the absorption of the light drops, and the TCO becomes transparent, since the dielectric function of the plasma gas is real [46, 47]. For wavelengths larger than the plasma wavelength, the dielectric function is imaginary, and the reflectivity of the TCO increases [48]. TCOs exhibit high transparency for
2. Transparent photodetector

Typical examples of TCOs are zinc oxide (ZnO), tin oxide (SnO$_2$) and indium oxide (In$_2$O$_3$). Indium tin oxide (ITO) or In$_2$O$_3$ doped with SnO$_2$ is a widely used TCO due to its high electrical conductivity. However, ITO is very expensive, and the film thickness has to be small to achieve sufficient transparency. ZnO and SnO$_2$ are cheap alternatives with good optical and moderate electrical properties. The energy band gaps of intrinsic ZnO and SnO$_2$ are 3.3 eV and 3.6 eV, respectively [49]. The optical and electrical properties of TCOs are tailored by doping. ZnO films are typically doped with aluminum (Al), gallium (Ga) or boron (B), while SnO$_2$ can be doped with indium (In) or fluorine (F). To depict the absorption properties of aluminum doped zinc oxide (ZnO:Al) deposited by radio frequency (RF) magnetron sputtering and fluorine doped tin oxide (SnO$_2$:F) deposited by atmospheric pressure chemical vapor deposition (APCVD), their absorption coefficients are adapted from the literature [41, 45].

Figure 2.2b shows that the absorption coefficient of sputtered ZnO:Al is larger than for APCVD SnO$_2$:F. However, for the spectrometer and interferometer applications based on sampling of a standing wave, it is necessary that the transparent photodetector exhibits flat interfaces so that the standing wave can be formed. Sputtered ZnO films deposited on a glass substrate exhibit smooth surface [50]. On the other hand, the surface of APCVD SnO$_2$ films is textured [51, 52]. Therefore, for the fabrication of the transparent photodetectors sputtered ZnO:Al is used [19, 35], while APCVD SnO$_2$:F is used in solar cell applications to introduce light trapping [51, 52].

2.2.3 Fabrication of transparent p-i-n photodiode

Stiebig et al. developed transparent p-i-n photodiode with a-Si:H as the active material [19, 35]. The optical properties of the a-Si:H limit the operating range of the transparent photodetector to the visible region of electromagnetic spectrum (Fig. 2.2a). The a-Si:H p-i-n photodiode is sandwiched between ZnO:Al transparent electrodes.

The first step in the fabrication of the transparent photodetector is deposition of the front ZnO:Al electrode on a glass substrate by RF magnetron sputtering. To
2.3 Analytical modeling of electromagnetic wave propagation

Figure 2.3: Transparent photodetectors with ultra thin layers.

realize ZnO:Al film, the sputtering deposition is done at a temperature of 400 °C [19, 35]. The a-Si:H p-i-n photodiode is deposited on the front ZnO:Al layer starting from the n-layer. The deposition of the p-i-n diode is realized in a multi-chamber plasma enhanced chemical vapor deposition (PECVD) system at 210 °C in a gas mixture of silane and hydrogen [19, 35]. The p- and n-type layers are deposited by adding trimethylboron and phosphine to the gas mixture, respectively [53].

The back ZnO:Al electrode is sputtered at room temperature to prevent damaging the a-Si:H p-i-n photodiode [19]. Photolithography and reactive ion etching are used to pattern the multilayer stack glass/ZnO_{F}/n-i-p/ZnO_{B}, and the realized transparent photodetectors exhibit an area of 10 mm² [19, 35]. To achieve high transmission, the total thickness of the p-i-n photodiode has to be less than 100 nm. Due to the small thickness of p-i-n photodiode, special efforts are needed to avoid shunting problems. The thickness of the ZnO:Al electrodes is sufficiently large to achieve good conductivity, but not too large to affect the antireflection properties [19]. The thickness of ZnO:Al transparent electrodes and the thickness of the p-i-n diode are optimized so that the transparent photodetector exhibits the maximum of the transmission for a wavelength of 633 nm [19]. The realized transparent p-i-n photodiodes are shown in Fig. 2.3.

2.3 Analytical modeling of electromagnetic wave propagation

The performances of optoelectronic devices can be modeled by determining the light propagation within the device. The light propagation is described by Maxwell’s equations. Maxwell’s equations establish the relationship between the electric and magnetic component of an electromagnetic wave. By solving Maxwell’s equations, the distribution of the electric and magnetic component is obtained, and the optoelectronic device can be fully characterized. For devices with simple multilayer structure and flat interfaces, analytical methods can be used to solve Maxwell’s equations. However, for devices with complex structure or textured interfaces, analytical methods will
result in a solution with low accuracy. The appearance of modern day computers has
initiated a development of different numerical methods to solve Maxwell’s equations.
Nowadays, due to the increasing processing power of computers, standard personal
computers can be used to implement numerical methods.

In this section, basic electromagnetic theory is presented. Analytical methods
used to model light propagation through simple devices with optically thin or thick
multilayer stacks are derived.

2.3.1 Electromagnetics theory - basics

Maxwell’s equations. Maxwell’s equations are a set of four equations that connect
the electric and magnetic component of an electromagnetic field. Maxwell’s equations
in differential form are given by [54–57]:

\[ \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \] (2.14)
\[ \nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} \] (2.15)
\[ \nabla \cdot \mathbf{D} = \rho \] (2.16)
\[ \nabla \cdot \mathbf{B} = 0 \] (2.17)

where \( \mathbf{J} \) is the electrical current density, \( \mathbf{E} \) is the electric field, \( \mathbf{H} \) is the magnetic field,
\( \mathbf{D} \) is the electric flux density, \( \mathbf{B} \) is the magnetic flux density, and \( \rho \) is the electric charge
density. Maxwell’s equations are accompanied by relationships that characterize the
material through which the electromagnetic wave is propagating:

\[ \mathbf{D} = \varepsilon_0 \varepsilon_r \mathbf{E} \] (2.18)
\[ \mathbf{B} = \mu_0 \mu_r \mathbf{H} \] (2.19)

where \( \varepsilon_0 \) is the dielectric permittivity of vacuum, \( \varepsilon_r \) is the relative dielectric permittivity
of the material, \( \mu_0 \) is the magnetic permeability of vacuum, and \( \mu_r \) is the relative
magnetic permeability of the material. For most materials, the relative magnetic
permeability is unity (\( \mu_r = 1 \)) in the visible region of the electromagnetic spectrum
[54–57].

For the electric and magnetic components of the electromagnetic wave that are
relatively small, the nonlinear effects in semiconductors can be neglected. Under these
conditions, following approximations are valid [54–57]:

\[ \mathbf{J} = \sigma \mathbf{E} \] (2.20)
\[ \rho = 0 \] (2.21)

where \( \sigma \) is conductivity of the semiconductor. Maxwell’s equations for semiconductors
are given by:

\[ \nabla \times \mathbf{E} = -\mu_0 \frac{\partial \mathbf{H}}{\partial t} \] (2.22)
2.3 Analytical modeling of electromagnetic wave propagation

\[ \nabla \times \mathbf{H} = \varepsilon_0 \varepsilon_r \frac{\partial \mathbf{E}}{\partial t} + \sigma \mathbf{E} \quad (2.23) \]

\[ \nabla \cdot \mathbf{E} = 0 \quad (2.24) \]

\[ \nabla \cdot \mathbf{H} = 0 \quad (2.25) \]

Wave equation. Wave equation is a simplified form of Maxwell’s equations defined only for the electric or magnetic component of an electromagnetic wave. Here, a wave equation for the magnetic field is derived. For this derivation it is necessary to take a curl of Eq. (2.23), which gives:

\[ \nabla \times \nabla \times \mathbf{H} = \varepsilon_0 \varepsilon_r \frac{\partial}{\partial t} (\nabla \times \mathbf{E}) + \sigma (\nabla \times \mathbf{E}) \quad (2.26) \]

By applying the relationship between electric and magnetic component (Eq. (2.22)), Eq. (2.26) becomes:

\[ \nabla \times \nabla \times \mathbf{H} = -\mu_0 \varepsilon_0 \varepsilon_r \frac{\partial^2 \mathbf{H}}{\partial t^2} - \mu_0 \sigma \frac{\partial \mathbf{H}}{\partial t} \quad (2.27) \]

To finalize the derivation, the vector identity \( \nabla \times \nabla \times \mathbf{a} = \nabla (\nabla \cdot \mathbf{a}) - \nabla^2 \mathbf{a} \) and Eq. (2.25) are applied:

\[ \nabla^2 \mathbf{H} - \mu_0 \sigma \frac{\partial \mathbf{H}}{\partial t} - \mu_0 \varepsilon_0 \varepsilon_r \frac{\partial^2 \mathbf{H}}{\partial t^2} = 0 \quad (2.28) \]

Equation (2.28) represents the wave equation for the magnetic component of the electromagnetic wave. The wave equation for the electric component is analogous:

\[ \nabla^2 \mathbf{E} - \mu_0 \sigma \frac{\partial \mathbf{E}}{\partial t} - \mu_0 \varepsilon_0 \varepsilon_r \frac{\partial^2 \mathbf{E}}{\partial t^2} = 0 \quad (2.29) \]

The solution of Eqs. (2.28) and (2.29) can be expressed as superposition of the monochromatic plane waves:

\[ \mathbf{a} = \mathbf{a}_0 e^{i(\omega t - kr)} \quad (2.30) \]

where \( \mathbf{a} \) is either an electric (\( \mathbf{E} \)) or a magnetic (\( \mathbf{H} \)) component, \( \mathbf{a}_0 \) is the respective amplitude, \( \omega \) is the angular frequency and \( \mathbf{k} \) is the wave vector of the electromagnetic wave, \( t \) is time, and \( \mathbf{r} \) is a position vector. By replacing the solution for electric and magnetic component, the complex form of Maxwell’s equations is obtained:

\[ \mathbf{k} \times \mathbf{E} = \omega \mu_0 \mathbf{H} \quad (2.31) \]

\[ \mathbf{k} \times \mathbf{H} = -\omega \varepsilon_0 \varepsilon_r \mathbf{E} + i\sigma \mathbf{E} \quad (2.32) \]

\[ \mathbf{k} \cdot \mathbf{E} = 0 \quad (2.33) \]

\[ \mathbf{k} \cdot \mathbf{H} = 0 \quad (2.34) \]
Equations (2.33) and (2.34) show that the wave vector is orthogonal to the electric and magnetic component of the electromagnetic wave. The intensity of the wave vector is given by [54–57]:

\[
k = \frac{2\pi}{\lambda} N = \frac{\omega}{c} N \tag{2.35}
\]

where \( \lambda \) is the wavelength of the electromagnetic wave, \( c \) is the speed of light, and \( N \) is the complex refractive index of the material.

The complex refractive index depends on the dielectric function and conductivity of the materials. This relationship can be established by replacing the solution of Eq. (2.30) into the wave equations (Eqs. (2.28) or (2.29)):

\[
k^2 E + i \omega \mu_0 \sigma E - \omega^2 \mu_0 \epsilon_0 E = 0 \tag{2.36}
\]

From Eqs. (2.35) and (2.36), the complex refractive index is given by:

\[
N^2 = \epsilon_r - i \frac{\sigma}{\omega \epsilon_0} \tag{2.37}
\]

where the expression for the speed of light in vacuum \( (c = \frac{1}{\sqrt{\mu_0 \epsilon_0}}) \) is applied.

**Poynting’s theorem and light intensity.** Poynting’s theorem establishes conservation of energy for the electromagnetic wave. The energy conservation law can be derived from Maxwell’s curl equations (Eqs. (2.22) and (2.23)). In the absence of current sources, the integral form of Poynting’s theorem is given by [54–57]:

\[
-\frac{\partial}{\partial t} \int_V \left( \frac{1}{2} \epsilon_0 \epsilon_r |E|^2 + \frac{1}{2} \mu_0 |H|^2 \right) \, dV = \oint_A (E \times H) \cdot d\mathbf{A} + \int_V (\sigma |E|^2) \, dV \tag{2.38}
\]

where \( V \) is an arbitrary volume enclosed by a surface \( A \) with a surface normal \( d\mathbf{A} \). Poynting’s theorem states that the decrease of the electromagnetic energy stored inside volume \( V \) is equal to the sum of the energy that leaves the volume through the surface \( A \) and the energy that is dissipated inside volume \( V \) due to the interaction of the electric field with charge carriers. According to Poynting’s theorem, the flow of the electromagnetic energy is defined by the vector:

\[
\mathbf{S} = \mathbf{E} \times \mathbf{H} \tag{2.39}
\]

which is called the Poynting vector. The Poynting vector can be interpreted as the power transferred by the electromagnetic wave per unit area. The direction of the Poynting vector is the same as that of the wave vector and represents the direction of the electromagnetic wave propagation.

The time-averaged magnitude of the Poynting vector is the light intensity (irradiance):

\[
I \equiv \frac{1}{T_{\text{per}}} \int_0^{T_{\text{per}}} |\mathbf{S}| \, dt \tag{2.40}
\]

where \( T_{\text{per}} \) is the period of the optical cycle. In the case of monochromatic plane waves where the electric and magnetic component are defined by Eq. (2.30), the light intensity (irradiance) is given by [56, 57]:

\[
I = \frac{1}{2} |\text{Re} (\mathbf{E} \times \mathbf{H}^*)| \tag{2.41}
\]
where $\mathbf{H}^*$ is complex conjugate of the magnetic component $\mathbf{H}$. The light intensity can be calculated from the electric or magnetic component of the electromagnetic wave. Here, the expression to calculate the light intensity from the magnetic component is derived. Starting from Eqs. (2.32), (2.35) and (2.37), the electric component can be expressed by using magnetic component:

$$\mathbf{E} = \frac{\mu_0 \omega \mathbf{H} \times \mathbf{k}}{k^2}$$

(2.42)

where vector identity $\mathbf{a} \times \mathbf{b} = -\mathbf{b} \times \mathbf{a}$ is used. By replacing Eq. (2.42) into Eq. (2.41), the light intensity becomes:

$$I = \frac{1}{2} \frac{\mu_0 \omega}{\text{Re}(k^2)} |\text{Re}(\mathbf{H} \times \mathbf{k} \times \mathbf{H}^*)|$$

(2.43)

By applying the vector identity $\mathbf{a} \times \mathbf{b} \times \mathbf{c} = \mathbf{b} (\mathbf{a} \cdot \mathbf{c}) - \mathbf{c} (\mathbf{a} \cdot \mathbf{b})$ and taking into account Eq. (2.34), the expression for the light intensity can be rewritten as:

$$I = \frac{1}{2} \frac{\mu_0 \omega \text{Re}(k)}{\text{Re}(k^2)} |\mathbf{H}|^2$$

(2.44)

Taking into account the definitions of the wave vector intensity (Eq. (2.35)) and complex refractive index (Eq. (2.2)), the light intensity can be expressed as:

$$I = \frac{1}{2} \frac{\mu_0 c \eta}{(\eta^2 + \kappa^2)} |\mathbf{H}|^2$$

(2.45)

To calculate the light intensity from the electric field component, the derivation starts from Eq. (2.31). In this case, the expression for the light intensity is given by:

$$I = \frac{1}{2} \epsilon_0 c \eta |\mathbf{E}|^2$$

(2.46)

In this study, Eq. (2.46) is used to calculate the light intensity. Therefore, when solving Maxwell’s equations, the goal is to obtain the electric component of the electromagnetic field.

**Reflection, refraction and Fresnel’s coefficients.** The laws of reflection and refraction combined with Fresnel coefficients describe the behavior of the electromagnetic wave at the interface between two materials. When crossing from one media to another, part of the input electromagnetic wave is reflected at the interface, and part of it passes through. The directions of the reflected and transmitted (refracted) wave are described by the laws of the reflection and refraction. Fresnel’s coefficients establish a connection between the amplitudes of the electric and magnetic component for the input, reflected and transmitted wave.

Figure 2.4 schematically depicts an incident ($i$), reflected ($r$) and transmitted ($t$) electromagnetic wave. In the case of the monochromatic plane waves, the direction of the wave propagation is described by the wave vector as shown in Fig. 2.4. The wave vectors of the incident, reflected and transmitted wave are in the same plane called the plane of incidence [56, 57]. The angles between the wave vector and interface normal for incident ($\theta_i$), reflected ($\theta_r$) and transmitted wave ($\theta_t$) are related by the laws of reflection and refraction. To derive these laws, boundary conditions for the electric
component of the electromagnetic wave have to be used. The boundary conditions state that projections of the electric field on the interface plane have to be equal at both sides of the interface [56, 57]:

\[ E_{i\tau} e^{i(\omega t - k_\tau r)} + E_{r\tau} e^{i(\omega t - k_\tau r)} = E_{t\tau} e^{i(\omega t - k_\tau r)} \] (2.47)

where position vector \( \mathbf{r} \) is now parallel to the interface plane. For Eq. (2.47) to be valid at any time and position, following conditions have to be satisfied:

\[ \omega_i = \omega_r = \omega_t \] (2.48)

\[ k_{i\tau} = k_{r\tau} = k_{t\tau} \] (2.49)

where \( k_{i\tau}, k_{r\tau} \) and \( k_{t\tau} \) are projections of the wave vector on the interface plane for incident, reflected and transmitted wave, respectively. By replacing Eq. (2.35) into Eq. (2.49), the laws of reflection and refraction are obtained:

\[ \theta_i = \theta_r \] (2.50)

\[ N_1 \sin \theta_i = N_2 \sin \theta_t \] (2.51)

The relation given by Eq. (2.51) is called Snell’s law. Snell’s law and reflection law are valid for any arbitrary polarization of the incident plane wave [56, 57].

Figure 2.5 depicts incident, reflected and transmitted plane wave for transverse electric (TE) and transverse magnetic (TM) polarization. Components orthogonal to the plane of incidence marked with symbol \( \odot \) have direction towards the viewer, while symbol \( \oplus \) is used for opposite direction. The connection between amplitudes of the electric field depends on the polarization of the incident electromagnetic plane wave, as stated by Eq. (2.47). For different polarizations of the plane wave, projections of the electric field on the interface plane are different. However, every polarization of the plane wave can be expressed as a superposition of TE and TM polarization [56, 57]. TE or orthogonal polarization is polarization of the plane wave where the electric field is orthogonal to the plane of incidence as shown in Fig. 2.5a. TM or parallel polarization occurs when the electric field is parallel to the plane of incidence, which is depicted in Fig. 2.5b.
2.3 Analytical modeling of electromagnetic wave propagation

Figure 2.5: Schematic representation of electric and magnetic component of the electromagnetic plane wave for (a) transverse electric and (b) transverse magnetic polarization.

Fresnel reflection coefficient is defined as the ratio between the reflected and incident wave:

\[ r = \frac{E_r}{E_i} \]  

(2.52)

On the other hand, Fresnel transmission coefficient is given by the ratio of transmitted and incident wave:

\[ t = \frac{E_t}{E_i} \]  

(2.53)

To derive Fresnel’s coefficients, the boundary conditions for the amplitudes of electric and magnetic component are used:

\[ a_{ir} + a_{rr} = a_{tr} \]  

(2.54)

where \( a_{ir}, a_{rr} \) and \( a_{tr} \) are amplitude projections of the electric \((a = E)\) or magnetic field \((a = H)\) on the interface plane for incident, reflected and transmitted wave, respectively. For TE polarization, Eq. (2.54) can be rewritten:

\[ E_{i\perp} + E_{r\perp} = E_{t\perp} \]  

(2.55)

\[ H_{i\parallel} \cos \theta_1 - H_{r\parallel} \cos \theta_1 = H_{t\parallel} \cos \theta_2 \]  

(2.56)

By using Eqs. (2.31) and (2.35), the parallel component of the magnetic field can be expressed as:

\[ H_{\parallel} = \frac{N}{c\mu_0}E_{\perp} \]  

(2.57)

Analogous relationship is valid for parallel electric and orthogonal magnetic field in TM polarization. After replacing Eq. (2.57) into Eq. (2.56), the boundary conditions for TE polarization become:

\[ E_{i\perp} + E_{r\perp} = E_{t\perp} \]  

(2.58)
By combining Eqs. (2.58) and (2.59) with Eqs. (2.52) and (2.53), Fresnel’s coefficients for TE polarization are obtained:

\[ r_\perp = \frac{N_1 \cos \theta_1 - N_2 \cos \theta_2}{N_1 \cos \theta_1 + N_2 \cos \theta_2} \tag{2.60} \]
\[ t_\perp = \frac{2N_1 \cos \theta_1}{N_1 \cos \theta_1 + N_2 \cos \theta_2} \tag{2.61} \]

For TM polarization, the boundary conditions are given by:

\[ E_{i\parallel} \cos \theta_1 + E_{r\parallel} \cos \theta_1 = E_{t\parallel} \cos \theta_2 \tag{2.62} \]
\[ N_1 E_{i\parallel} - N_1 E_{r\parallel} = N_2 E_{t\parallel} \tag{2.63} \]

where magnetic field components are replaced by electric field using relationship which is analogous to Eq. (2.57). From Eqs. (2.62) and (2.63), Fresnel’s coefficients for TM polarization are obtained:

\[ r_\parallel = \frac{N_1 \cos \theta_2 - N_2 \cos \theta_1}{N_1 \cos \theta_2 + N_2 \cos \theta_1} \tag{2.64} \]
\[ t_\parallel = \frac{2N_1 \cos \theta_1}{N_1 \cos \theta_2 + N_2 \cos \theta_1} \tag{2.65} \]

Fresnel’s coefficients are used to determine the reflection and transmission of the light at the interface between two materials [56, 57]:

\[ R = \frac{I_r}{I_i} = |r|^2 \tag{2.66} \]
\[ T = \frac{I_t}{I_i} = \frac{\eta_2 \cos \theta_2}{\eta_1 \cos \theta_1} |t|^2 \tag{2.67} \]

where \( I_i, I_r \) and \( I_t \) are intensities of the incident, reflected and transmitted plane wave, respectively.

### 2.3.2 Thin-film optics

Thin-film optics models the propagation of the light in nano-structured layers of different materials with flat interfaces. In order to apply thin-film optics, the thicknesses of the layers have to be comparable to the wavelength of the light. At such scales, electromagnetic waves that pass through the thin-film layers exhibit interference effects. Interference is a phenomenon in which electromagnetic waves of the same wavelength superimpose to produce a new wave [54–56]. The intensity of the resulting wave is given by [54–56]:

\[ I = I_1 + I_2 + 2\sqrt{I_1I_2} \cos \varphi \tag{2.68} \]

where \( I_1 \) and \( I_2 \) are the intensities of the interfering waves, and \( \varphi \) is the phase difference between them. In thin-films, interference occurs between electromagnetic waves that are reflected or transmitted at the interfaces between different materials.
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Figure 2.6: Schematic representation of a layer stack and elements of transfer matrix method for thin-films.

The thin-film interference effect is typically used to enhance reflection or transmission properties of the nano-structured layers. This is achieved by utilizing materials with specific optical properties and by tuning the number of layers and their thickness. The electromagnetic wave in the structure with numerous thin-film layers exhibits multiple reflections and transmissions at interfaces between different materials. Consequently, the thin-film interference is an interference of multiple electromagnetic waves. To describe the electromagnetic wave propagation under such conditions, a transfer matrix method can be used. The transfer matrix method combines Fresnel’s coefficients, the laws of reflection and refraction, and the wave propagation through the thin-film layers. The transfer matrix method is demonstrated for multilayer structure (Fig. 2.6).

Figure 2.6 schematically depicts a multilayer stack that consists of \((n)\) layers. Each layer is a homogenous material with defined thickness \((d)\) and described by the complex refractive index \((N)\). The input media has to be non-absorbing, which can be achieved by using only the real part of the complex refractive index. The input (layer \((0)\)) and exit media (layer \((n+1)\)) are assumed to be infinitely thick, and they are characterized only by the refractive index \((N_0, N_{n+1})\). To simplify the derivation, the incident electromagnetic plane wave is normal to the layer stack, and the direction of the wave propagation is denoted with \(z\)-axis. For the normal incidence, Fresnel’s coefficients for TE and TM polarization at the interface between layers \((j)\) and \((j+1)\) are equal and given by:

\[
\begin{align*}
    r_{j,j+1} &= \frac{N_j - N_{j+1}}{N_j + N_{j+1}} \\
    t_{j,j+1} &= \frac{2N_j}{N_j + N_{j+1}}
\end{align*}
\]  

Under the normal incidence, the laws of reflection and refraction state that the reflected and transmitted wave travel along the same path, but in opposite direction. Plane waves transmitted through the layer interfaces propagate in positive direction, and they are marked with \((+)\). On the other hand, plane waves reflected at the interface propagate in negative direction, and they are marked with \((-)\). Electric fields in Fig. 2.6 are indexed by the layer in which they are present and by the neighboring
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Layer that forms the interface.

Transfer matrix method establishes a connection between electric field components at layer interfaces. According to Eqs. (2.58), (2.59), (2.62) and (2.63), the boundary conditions at the interface between layers (j-1) and (j) can be expressed as:

\[ E_{j-1,j}^+ + E_{j-1,j}^- = E_{j,j-1}^+ + E_{j,j-1}^- \]  (2.71)

\[ N_{j-1} E_{j-1,j}^+ - N_{j-1} E_{j-1,j}^- = N_j E_{j,j-1}^+ - N_j E_{j,j-1}^- \]  (2.72)

By using Eqs. (2.69) and (2.70), the boundary conditions are transformed into:

\[ E_{j-1,j}^+ = \frac{1}{t_{j-1,j}} E_{j,j-1}^+ + \frac{r_{j-1,j}}{t_{j-1,j}} E_{j,j-1}^- \]  (2.73)

\[ E_{j-1,j}^- = \frac{r_{j-1,j}}{t_{j-1,j}} E_{j,j-1}^+ + \frac{1}{t_{j-1,j}} E_{j,j-1}^- \]  (2.74)

or in matrix notation:

\[
\begin{bmatrix}
E_{j-1,j}^+ \\
E_{j-1,j}^-
\end{bmatrix} =
\begin{bmatrix}
\frac{1}{t_{j-1,j}} & \frac{r_{j-1,j}}{t_{j-1,j}} \\
\frac{r_{j-1,j}}{t_{j-1,j}} & \frac{1}{t_{j-1,j}}
\end{bmatrix}
\begin{bmatrix}
E_{j,j-1}^+ \\
E_{j,j-1}^-
\end{bmatrix}
\] (2.75)

Propagation conditions within layer (j) establish connection between electric field components at interfaces with layer (j-1) and layer (j+1):

\[ E_{j,j-1}^+ = E_{j,j+1}^+ \exp(i\phi_j) \]  (2.76)

\[ E_{j,j-1}^- = E_{j,j+1}^- \exp(-i\phi_j) \]  (2.77)

where \( \phi_j \) is the phase thickness of layer (j), and it is given by:

\[ \phi_j = \frac{2\pi}{\lambda} N_j (z_j - z_{j-1}) = \frac{2\pi}{\lambda} N_j d_j \]  (2.78)

The propagation conditions can be expressed in matrix notation:

\[
\begin{bmatrix}
E_{j,j-1}^+ \\
E_{j,j-1}^-
\end{bmatrix} =
\begin{bmatrix}
\exp(i\phi_j) & 0 \\
0 & \exp(-i\phi_j)
\end{bmatrix}
\begin{bmatrix}
E_{j,j+1}^+ \\
E_{j,j+1}^-
\end{bmatrix}
\] (2.79)

By combining Eqs. (2.75) and (2.79), a connection between electric field components at layer (j) interfaces is established:

\[
\begin{bmatrix}
E_{j-1,j}^+ \\
E_{j-1,j}^-
\end{bmatrix} =
\begin{bmatrix}
\frac{1}{t_{j-1,j}} \exp(i\phi_j) & \frac{r_{j-1,j}}{t_{j-1,j}} \exp(-i\phi_j) \\
\frac{r_{j-1,j}}{t_{j-1,j}} \exp(i\phi_j) & \frac{1}{t_{j-1,j}} \exp(-i\phi_j)
\end{bmatrix}
\begin{bmatrix}
E_{j,j+1}^+ \\
E_{j,j+1}^-
\end{bmatrix}
\] (2.80)

Reflection and transmission coefficients at interface between layers (j) and (j+1) are defined as:

\[ \tilde{r}_{j,j+1} = \frac{E_{j,j+1}^-}{E_{j,j+1}^+} \]  (2.81)

\[ \tilde{t}_{j,j+1} = \frac{E_{j+1,j}^+}{E_{j,j+1}^+} \] (2.82)
At the interface between layers (j-i) and (j), reflection and transmission coefficients are derived from Eqs. (2.79), (2.80) and (2.81):

\[
\tilde{r}_{j-1,j} = \frac{E_{j-1,j}^+}{E_{j-1,j}^-} = \frac{r_{j-1,j} + \tilde{r}_{j,j+1} \exp(-i2\phi_j)}{1 + r_{j-1,j} \tilde{r}_{j,j+1} \exp(-i2\phi_j)} \quad (2.83)
\]

\[
\tilde{t}_{j-1,j} = \frac{E_{j-1,j}^+}{E_{j-1,j}^-} = \frac{t_{j-1,j}}{1 + r_{j-1,j} \tilde{r}_{j,j+1} \exp(-i2\phi_j)} \quad (2.84)
\]

From Eqs. (2.80), (2.82) and (2.84), a transmission coefficient between layers (j-1) and (j+1) can be derived:

\[
\tilde{t}_{j-1,j+1} = \frac{E_{j+1,j}^+}{E_{j+1,j}^-} = \tilde{t}_{j-1,j} \exp(-i\phi_j) \tilde{t}_{j,j+1} \quad (2.85)
\]

Finally, generalization of Eqs. (2.83), (2.84) and (2.85) gives:

\[
\tilde{r}_{j,j+1} = \frac{r_{j,j+1} + \tilde{r}_{j,j+2} \exp(-i2\phi_{j+1})}{1 + r_{j,j+1} \tilde{r}_{j,j+2} \exp(-i2\phi_{j+1})} \quad (2.86)
\]

\[
\tilde{t}_{j,j+1} = \frac{t_{j,j+1}}{1 + r_{j,j+1} \tilde{r}_{j,j+2} \exp(-i2\phi_{j+1})} \quad (2.87)
\]

\[
\tilde{t}_{0,j} = \tilde{t}_{0,1} \exp(-i\phi_1) \tilde{t}_{1,2} \cdots \tilde{t}_{j-2,j-1} \exp(-i\phi_{j-2}) \tilde{t}_{j-1,j} \quad (2.88)
\]

Recurrent calculation of transmission and reflection coefficients for thin-film layers starts from interface between layers (n) and (n+1) where Fresnel’s coefficients are used:

\[
\tilde{r}_{n,n+1} = r_{n,n+1} \quad (2.89)
\]

\[
\tilde{t}_{n,n+1} = t_{n,n+1} \quad (2.90)
\]

Total reflectivity and transmission of the thin-film layer stack are given by:

\[
R = \frac{I_{0,1}^-}{I_{0,1}^+} = |\tilde{r}_{0,1}|^2 \quad (2.91)
\]

\[
T = \frac{I_{n+1,0}^+}{I_{n+1,0}^-} = \frac{\eta_{n+1}}{\eta_0} |\tilde{t}_{0,n+1}|^2 \quad (2.92)
\]

where Eq. (2.46) is used for the corresponding light intensities. For a multilayer stack with inverted order of layers where layer (n+1) is the input and layer (0) is the exit media, transmission remains the same (\(T_{inverted} = T\)), but reflectivity is different (\(R_{inverted} \neq R\)) [58]. The derived equations are also valid for different angles of incidence. For such a case, the reflection and transmission coefficients are replaced by the corresponding Fresnel’s coefficients for TE or TM polarization. Also, for the phase thickness (Eq. (2.78)) and total transmission (Eq. (2.92)), the effective refractive index has to be used:

\[
N_{j}^{eff} = N_j \cos \theta_j \quad (2.93)
\]

where \(\theta_j\) is the refraction angle for layer (j) given by Snell’s law (\(N_0 \sin \theta_0 = N_1 \sin \theta_1 = \cdots = N_j \sin \theta_j = \cdots = N_{n+1} \sin \theta_{n+1}\)).
To fully characterize optoelectronic devices with thin-film layers, it is important to determine the electric field distribution within its layers. Within layer \((j)\), the electric field is superposition of the forward and backward propagating plane wave:

\[
E_j(z) = E_{j,j-1}^+ \exp(-ik_j(z - z_{j-1})) + E_{j,j+1}^- \exp(ik_j(z - z_{j-1} - d_j))
\]  
(2.94)

where \(z \in (z_{j-1}, z_j)\). By using the propagation conditions (Eq. (2.79)), definition of the reflection coefficient (Eq. (2.81)) and transmission coefficient between layers \((0)\) and layer \((j)\) (Eq. (2.88)), Eq. (2.94) can be rewritten into:

\[
E_j(z') = E_{0,1}^+ \tilde{r}_{0,j} \left( \exp(-ik_j z') + \tilde{r}_{j,j+1} \exp(-i2\phi_j) \exp(ik_j z') \right)
\]  
(2.95)

where \(z' = z - z_{j-1} \in (0, d_j)\). The intensity of the light in the layer \((j)\) is derived by replacing Eq. (2.95) into Eq. (2.46):

\[
I_j(z') = I_{0,1}^+ T_{0,j} \left( \exp(-\alpha_j z') + R_{j,j+1} \exp(-\alpha_j (2d_j - z')) + 2 \sqrt{I_{1} I_{2}} |g| \cos \left( \frac{4\pi}{\lambda} \eta_j (d_j - z') - \arg(\tilde{r}_{j,j+1}) \right) \right)
\]  
(2.96)

where \(\alpha_j\) is the absorption coefficient of layer \((j)\), \(R_{j,j+1}\) is the reflectivity of all layers behind layer \((j)\) \((R_{j,j+1} = |\tilde{r}_{j,j+1}|^2)\), \(T_{0,j}\) is the transmission from layer \((0)\) to layer \((j)\) \((T_{0,j} = \frac{n_j}{n_0} |\tilde{t}_{0,j}|^2)\), and \(\arg(\tilde{r}_{j,j+1})\) represents the phase of the reflection coefficient. Equation (2.96) is analogous to Eq. (2.68) and represents the intensity of the electromagnetic wave, which is the result of the interference between the forward and backward propagating wave in a thin-film multilayer stack.

**Non-interference films.** Monochromatic plane waves defined by Eq. (2.30) display predictable dependence on the time and position, and their behavior is deterministic. However, light sources usually consist of many atoms that radiate independently with slightly different frequencies and phases \([55, 56]\). Therefore, the produced light exhibits irregular fluctuations of the amplitude and the phase, which is not totally predictable \([55, 56]\).

The random fluctuations of the amplitude and phase influence the interference of the light. In order for light to interfere, it is necessary for electromagnetic waves that interact to exhibit sufficient correlation between their amplitudes and phases. Based on the degree of correlation, the light can be classified as coherent, partially coherent and non-coherent. The correlation between electromagnetic waves is defined by the mutual coherence function \((g)\) given by \([55, 56]\):

\[
g = \frac{E_1^* E_2}{\sqrt{I_1 I_2}} = |g| \exp(i\varphi)
\]  
(2.97)

where the amplitude of the mutual coherence function \((|g|)\) represent the degree of coherence, and the phase of the coherence function \((\varphi)\) represents the phase difference between the waves. The degree of correlation varies between zero and unity \((0 \leq |g| \leq 1)\). To account for the coherence of the light, the interference equation (Eq. (2.68)) can be modified into \([55, 56]\):

\[
I = I_1 + I_2 + 2\sqrt{I_1 I_2} |g| \cos \varphi
\]  
(2.98)
2.3 Analytical modeling of electromagnetic wave propagation

For coherent light, the degree of correlation is unity ($|g| = 1$), and Eq. (2.98) takes the form of Eq. (2.68). For non-coherent light, the degree of correlation is equal to zero ($|g| = 0$), and Eq. (2.98) becomes:

$$I = I_1 + I_2$$ (2.99)

In general, the degree of correlation can be described either by exponential or by Gaussian function [55, 56]. The exponential function can be used for the light with short coherence time, while the Gaussian function can used for the light with long coherence time. Coherence time represents time delay within which the random fluctuations are strongly correlated [56]. In this thesis, the degree of correlation is represented by Gaussian function assuming light sources with longer coherence time. Consequently, the degree of correlation is given by:

$$|g(\Delta L)| = \exp\left(-\frac{\pi \Delta L^2}{2L_c^2}\right)$$ (2.100)

where $\Delta L$ is the optical path difference between interfering waves, and $L_c$ is the coherence length (product of speed of light and coherence time). When the coherence length is much larger than the optical path difference ($L_c \gg \Delta L$), the degree of correlation tends to unity, and the light can be treated as coherent. On the other hand, the light becomes non-coherent if the optical path difference is much larger than the coherence length ($\Delta L \gg L_c$). In a layer stack, the optical path is proportional to the layer thicknesses. If the thickness of the layers is sufficiently large, the propagation of light through the layer stack will not be influenced by the interference effects. In this case, the light propagation is governed by the multiple reflections and additions of the light intensities. The light propagation in such a system can be modeled by using transfer matrix method for non-interference films.

Figure 2.7: Schematic representation of a layer stack and elements of transfer matrix method for non-interference films.
2. Transparent photodetector

Figure 2.7 depicts a layer stack that consists of (n) layers with elements used in transfer matrix calculations. The layers are sufficiently thick so that interference effects between forward and backward propagating wave within a layer can be neglected. Therefore, propagating waves are now described by the intensity and not by the electric field component. The description of layers, input and exit media, and denoting of the forward and backward propagating waves are the same as for the interference films case. Also, the input light is again of normal incidence to the layer stack and propagates along the \( z \)-axis. Interfaces between layers can be simple interface between two materials or a multilayer stack of thin-films. For the interface between layers \((j)\) and \((j+1)\), following relationships are valid in general case:

\[
R_{j,j+1} \neq R_{j+1,j} \quad (2.101)
\]

\[
T_{j,j+1} = T_{j+1,j} \quad (2.102)
\]

where reflectivities and transmissions of the interface are calculated from Eqs. (2.91) and (2.92), respectively, with layers \((j)\) and \((j+1)\) being input or exit media for the thin-film multilayer stack.

Transfer matrix method for non-interference films establishes a connection between intensities of the light at layer interfaces. Boundary conditions for the interface between layers \((j-1)\) and \((j)\) are given by:

\[
\begin{bmatrix}
I_{j,j-1}^+ & I_{j,j-1}^-
\end{bmatrix} =
\begin{bmatrix}
T_{j-1,j} & -R_{j-1,j}
T_{j-1,j}^2 & -R_{j-1,j}^2
\end{bmatrix}
\begin{bmatrix}
I_{j-1,j}^+ & I_{j-1,j}^-
\end{bmatrix} \quad (2.103)
\]

\[
\begin{bmatrix}
I_{j-1,j}^+ & I_{j-1,j}^-
\end{bmatrix} =
\begin{bmatrix}
T_{j-1,j} & -R_{j-1,j}
T_{j-1,j}^2 & -R_{j-1,j}^2
\end{bmatrix}
\begin{bmatrix}
I_{j-1,j}^+ & I_{j-1,j}^-
\end{bmatrix} \quad (2.104)
\]

which can be transformed into matrix notation:

\[
\begin{bmatrix}
I_{j-1,j}^+ & I_{j-1,j}^-
\end{bmatrix} =
\begin{bmatrix}
\frac{1}{T_{j-1,j}} & -\frac{R_{j-1,j}}{T_{j-1,j}^2}
\frac{R_{j-1,j}}{T_{j-1,j}} & \frac{T_{j-1,j}^2 - R_{j-1,j}^2}{T_{j-1,j}^2}
\end{bmatrix}
\begin{bmatrix}
I_{j-1,j}^+ & I_{j-1,j}^-
\end{bmatrix} \quad (2.105)
\]

where equality of transmissions given by Eq. (2.102) is used. The propagation conditions within layer \((j)\) are derived from the Beer-Lambert-Bouguer law (Eq. (2.9)) and can be written in matrix notation:

\[
\begin{bmatrix}
I_{j,j-1}^+ & I_{j,j-1}^-
\end{bmatrix} =
\begin{bmatrix}
\exp (\alpha d_j) & 0
0 & \exp (-\alpha d_j)
\end{bmatrix}
\begin{bmatrix}
I_{j,j+1}^+ & I_{j,j+1}^-
\end{bmatrix} \quad (2.106)
\]

The transfer matrix equation for non-interference films is obtained by combining Eqs. (2.105) and (2.106):

\[
\begin{bmatrix}
I_{j-1,j}^+ & I_{j-1,j}^-
\end{bmatrix} =
\begin{bmatrix}
\frac{1}{T_{j-1,j}} \exp (\alpha d_j) & -\frac{R_{j-1,j}}{T_{j-1,j}^2} \exp (\alpha d_j)
\frac{R_{j-1,j}}{T_{j-1,j}} \exp (\alpha d_j) & \frac{T_{j-1,j}^2 - R_{j-1,j}^2}{T_{j-1,j}^2} \exp (\alpha d_j)
\end{bmatrix}
\begin{bmatrix}
I_{j,j+1}^+ & I_{j,j+1}^-
\end{bmatrix} \quad (2.107)
\]

Total reflectivity and transmission at interface between layers \((j)\) and \((j+1)\) can be defined by:

\[
\tilde{R}_{j,j+1} = \frac{I_{j,j+1}^-}{I_{j,j+1}^+} \quad (2.108)
\]
The total reflectivity and transmission at the interface between layers (j-1) and (j), as well as the transmission from layer (j-1) to layer (j+1), are derived from Eqs. (2.106), (2.107), (2.108) and (2.109):

\[
\begin{align*}
\tilde{R}_{j-1,j} &= \frac{I_{j-1,j}^-}{I_{j-1,j}^+} = R_{j-1,j} + \frac{T_{j-1,j}^2 \tilde{R}_{j,j+1} \exp(-2\alpha_j d_j)}{1 - R_{j,j-1} \tilde{R}_{j,j+1} \exp(-2\alpha_j d_j)} \\
\tilde{T}_{j-1,j} &= \frac{I_{j-1,j}^+}{I_{j-1,j}^-} = \frac{T_{j-1,j}}{1 - R_{j,j-1} \tilde{R}_{j,j+1} \exp(-2\alpha_j d_j)} \\
\tilde{T}_{j-1,j+1} &= \frac{I_{j-1,j}^+}{I_{j-1,j}^-} = \tilde{T}_{j-1,j} \exp(-\alpha_j d_j) \tilde{T}_{j,j+1}
\end{align*}
\]

which can be generalized into:

\[
\begin{align*}
\tilde{R}_{j,j+1} &= R_{j,j+1} + \frac{T_{j,j+1}^2 \tilde{R}_{j+1,j+2} \exp(-2\alpha_{j+1} d_{j+1})}{1 - R_{j+1,j} R_{j+1,j+2} \exp(-2\alpha_{j+1} d_{j+1})} \\
\tilde{T}_{j,j+1} &= \frac{T_{j,j+1}}{1 - R_{j+1,j} \tilde{R}_{j+1,j+2} \exp(-2\alpha_{j+1} d_{j+1})} \\
\tilde{T}_{0,j} &= \tilde{T}_{0,1} \exp(-\alpha_1 d_1) \tilde{T}_{1,2} \cdots \tilde{T}_{j-2,j-1} \exp(-\alpha_{j-1} d_{j-1}) \tilde{T}_{j-1,j}
\end{align*}
\]

Recurrent calculations start from interface between layers (n) and (n+1), for which following relationships are valid:

\[
\begin{align*}
\tilde{R}_{n,n+1} &= R_{n,n+1} \\
\tilde{T}_{n,n+1} &= T_{n,n+1}
\end{align*}
\]

By using the transfer matrix model for non-interference films, the intensity within the layer (j) is a superposition of the forward and backward propagating wave intensities:

\[
I_j(z) = I_{j,j-1}^+ \exp(-\alpha_j (z - z_{j,min})) + I_{j,j+1}^- \exp(\alpha_j (z - z_{j,min} - d_j))
\]

where \(z \in (z_{j,min}, z_j)\). Equation (2.118) can be transformed into:

\[
I_j(z') = I_{0,1}^+ \tilde{T}_{0,j} \left( \exp(-\alpha_j z') + \tilde{R}_{j,j+1} \exp(-\alpha_j (2d_j - z')) \right)
\]

where \(z' = z - z_{j,min} \in (0, d_j)\). Equation (2.119) is analogous to Eq. (2.99) and can be also obtained from Eq. (2.96) by removing the interference element.

**Fabry-Perot resonator, absorption film and antireflection coating.** To establish a relationship between transfer matrix methods for interference and non-interference films, both methods are used to determine the total transmission \(T_{tot}\) of the light through a single film layer depicted in Fig. 2.8. In general, the optical properties of the thin-film, input and exit media shown in Fig. 2.8 are different. The
2. Transparent photodetector

Figure 2.8: Schematic representation of a single film layer.

Total transmission calculated by the transfer matrix method for interference films is given by:

\[
T_{\text{tot}}^I = \frac{\eta_2}{\eta_0} \left| \frac{t_{0,1} t_{1,2} \exp(-i\phi_1)}{1 + r_{0,1} r_{1,2} \exp(-i2\phi_1)} \right|^2
\]

while the transmission calculated by the non-interference method is given by:

\[
T_{\text{tot}}^{NI} = \frac{T_{0,1} T_{1,2} \exp(-\alpha_1 d_1)}{1 - R_{1,0} R_{1,2} \exp(-2\alpha_1 d_1)}
\]

Equation (2.122) shows that the transmission of the Fabry-Perot resonator is a periodic function of the air gap thickness \(d_1\). The air gap between glass sheets acts as a resonator. By changing its thickness, the transmission of the Fabry-Perot resonator can be tuned (Fig. 2.9).

Figure 2.9a exhibits the transmission of the Fabry-Perot resonator as the function of resonator (air gap) thickness for a wavelength of 600 nm calculated by Eqs. (2.122) and (2.123). When interference effects are present, a maximum of the transmission is achieved if the optical thickness of the resonator cavity is an integer multiple of half of the wavelength \(n_1 d_1 = n \cdot \lambda/2\). On the other hand, when interference effects are not present, the transmission is independent of the resonator thickness. Relationship between the total transmission calculated by interference and non-interference transfer matrix method is given by:

\[
T_{\text{tot}}^{NI} = \frac{T_{\text{tot}}^I}{T_{\text{tot}}^I}
\]
2.3 Analytical modeling of electromagnetic wave propagation

Transmission of the Fabry-Perot resonator as a function of resonator thickness for a wavelength of 600 nm using (a) interference and non-interference transfer matrix methods and (b) partially coherent model.

Figure 2.9: Transmission of the Fabry-Perot resonator as a function of resonator thickness for a wavelength of 600 nm using (a) interference and non-interference transfer matrix methods and (b) partially coherent model.

where $\overline{T_{tot}}$ is average value of $T_{tot}$ over one period ($\lambda/2$). Equation (2.124) can be proven by applying the integral identity

$$\frac{1}{2\pi} \int_0^{2\pi} \frac{d\beta}{a+b \cos \beta} = \frac{1}{\sqrt{a^2-b^2}}$$

to Eq. (2.122). By establishing a connection between transfer matrix models for interference and non-interference films, it is possible to define a model that accounts for the coherence of the light. Considering the interference equation for the partially coherent light (Eq. (2.98)) and definition of the degree of correlation (Eq. (2.100)), the total transmission of the Fabry-Perot resonator for partially coherent light ($T_{tot}^{PC}$) can be written as:

$$T_{tot}^{PC} = T_{tot}^{NI} + (T_{tot}^I - T_{tot}^{NI}) \exp \left( \frac{-2\pi n_0^2 d_1^2}{L_c^2} \right) \quad (2.125)$$

since the optical path difference is equal to twice the optical thickness of the resonator ($\Delta L = 2n_1 d_1$). The transmission of the Fabry-Perot resonator for partially coherent light with coherence lengths of 1 $\mu$m and 2 $\mu$m is shown in Fig. 2.9b. With increasing thickness of the resonator, the interference fringes disappear, and the total transmission is equal to the transmission for the non-interference case. Equation (2.125) is also applicable for the reflectivity of the Fabry-Perot resonator.

The connection between transfer matrix methods for interference and non-interference films (Eq. (2.124)) is also valid when the structure in Fig. 2.8 represents an absorption film or antireflection coating. The absorption film is a thin-film material deposited on a non-absorbing substrate. In this case, a silicon film deposited on a glass substrate with air as input media is analyzed ($N_0 = N_{air}$, $N_1 = N_{Si}$, $N_2 = N_{glass}$). The transmission through the silicon film is calculated by Eqs. (2.120) and (2.121), and it is depicted in Fig. 2.10 as a function of the film thickness.

Figure 2.10a shows that maximum of the transmission through the silicon film is achieved under the same conditions as for the Fabry-Perot resonator ($n_1d_1 = \eta \cdot \lambda/2$). Due to the absorption in the film, the amplitude of the interference fringes is reduced when increasing film thickness. The partially coherent model defined by Eq. (2.125) can also be applied for this case, and it is valid for the transmission, reflectivity and absorption of the silicon thin-film. The transmission through the silicon film for partially coherent light is shown in Fig. 2.10b. The interference fringes disappear...
due to the increased phase difference between the forward and backward propagating wave.

An antireflection coating is a thin-film material deposited at the interface between materials with low and high refractive index. In order to act as an antireflection coating, the value of the refractive index of the deposited material has to be within the range defined by the low and high refractive index materials ($N_0 < N_1 < N_2$). To demonstrate the principle of antireflection coatings, a case of ZnO film deposited on a silicon substrate with air as input media is analyzed ($N_0 = N_{air}$, $N_1 = N_{ZnO}$, $N_2 = N_{Si}$). The transmission through the ZnO film as a function of the film thickness is presented in Fig. 2.11.

Figure 2.11a shows that the connection established by Eq. (2.124) is also valid for this case. For the antireflection coating, the condition of maximum transmission requires that the optical thickness of the film is equal to an odd multiple of the quarter of the wavelength ($\eta_1 d_1 = (2n+1)\cdot\lambda/4$). Since the absorption in the ZnO film is small, the amplitude of interference fringes is not significantly reduced compared to the case of silicon film on a glass substrate. Partially coherent model is shown in Fig. 2.11b. Same behavior is observed as for the Fabry-Perot resonator and absorption film.

### 2.4 Optical model of transparent photodetector

Transparent photodetectors are ultra thin devices prepared on thick transparent substrates. To predict the optical performances of the transparent photodetector such as the transmission and quantum efficiency, an accurate model is required. Since the transparent photodetector is prepared on a flat glass substrate, the layer interfaces are also flat. Therefore, an accurate model of a transparent photodetector can be created by combining transfer matrix methods for interference and non-interference films. The propagation of the light through the thick substrate is described by the non-interference model. The transfer matrix method for interference films is used to model the light propagation through the thin-films that compose the transparent photodetector.
2.4 Optical model of transparent photodetector

As described previously (Sec. 2.2.3), the multilayer stack that composes the transparent photodetector consists of a thick glass substrate, front ZnO antireflection coating, p-i-n photodiode and back ZnO antireflection coating. Due to the asymmetry of the layer sequence, the quantum efficiency of the transparent photodetector depends on the direction from which the light enters the detector. Therefore, it is necessary to develop optical models of the detector when the light enters from the glass side and from the side of the back ZnO antireflection coating.

**Glass side.** The configuration of the transparent photodetector when the light enters from the glass side is presented in Fig. 2.12. The transparent photodetector is divided into two subsystems. The first subsystem is represented by the interface between air and the glass substrate, while the second is represented by a detector multilayer stack glass/ZnO$_F$/n-i-p/ZnO$_B$. Each of these subsystems is analyzed by a transfer matrix method for the interference films. The interaction between subsystems is described by non-interference transfer matrix method. Figure 2.12a depicts elements of the transfer matrix method for the non-interference films. Figure 2.12b depicts elements for interference transfer matrix method for the detector subsystem, where number indexing is replaced by layer names.

The transmission through the complete transparent photodetector is the ratio between the output intensity ($I_{out}$) and input intensity ($I_{in}$). Based on Eq. (2.121), the transmission is given by:

$$T_{tot} = \frac{T_{int} \cdot T_{det}}{1 - R_{int} \cdot R_{det}}$$  \hspace{1cm} (2.126)

where $R_{int}$ and $T_{int}$ are the reflectivity and transmission through the air/glass interface, and $R_{det}$ and $T_{det}$ are the reflectivity and transmission of the detector subsystem, respectively. For the detector subsystem, the reflectivity and transmission are calculated according to Eqs. (2.91) and (2.92) using interference transfer matrix elements $\tilde{r}_{glass,ZnO_F}$ and $\tilde{t}_{glass,air}$ (Fig. 2.12b).

The light intensity that enters the detector subsystem is given by $I'_{in}$. Between the interface and detector subsystem multiple non-interference reflections are occurring.
2. Transparent photodetector

![Diagram](image)

Figure 2.12: Modeling the transparent photodetector when light enters from the glass side. (a) The thick glass substrate is modeled with non-interference transfer matrix method, while (b) the transparent photodetector is modeled with interference transfer matrix method.

Therefore, the connection between \( I'_{in} \) and \( I_{in} \) is established by the non-interference transfer matrix method. The intensity of the light in the i-layer can be calculated according to Eq. (2.96). From the light intensity in the i-layer, the power loss profile (Eq. (2.8)) and photocurrent (Eq. (2.11)) are obtained. The photocurrent is used to determine the quantum efficiency according to Eq. (2.4):

\[
QE = \frac{T_{int}T_{glass,i}}{1 - R_{int}R_{det}} \left( 1 - \exp(-\alpha_i d_i) + R_{i,p} \exp(-\alpha_i d_i) - R_{i,p} \exp(-2\alpha_i d_i) + \frac{4\kappa_i^\prime}{\eta_i} \sqrt{R_{i,p}} \exp(-\alpha_i d_i) \sin\left(\frac{2\pi}{\lambda} \eta_i d_i\right) \cos\left(\frac{2\pi}{\lambda} \eta_i d_i - \arg(\tilde{r}_{i,p})\right)\right) \tag{2.127}
\]

where \( R_{i,p} \) is the reflectivity of all layers behind the i-layer, and \( T_{glass,i} \) is the transmission from the glass substrate into the i-layer. To determine the reflectivity behind the i-layer and transmission into the i-layer, interference transfer matrix elements \( \tilde{r}_{i,p} \) and \( \tilde{t}_{glass,i} \) are used (Fig. 2.12b).

**Back ZnO side.** When light enters the transparent photodetector from the back ZnO electrode, it first propagates through the detector and then through the interface subsystem. The configuration of the transparent photodetector for this case is shown in Fig. 2.13. Figure 2.13a depicts elements of the transfer matrix method for the non-interference films. Due to the multiple non-interference reflections in the glass substrate between the detector and interface subsystem, part of the light (\( I_{bn} \)) is reflected back entering the detector subsystem from the glass substrate. Therefore, for this configuration it is necessary to use transfer matrix elements for both directions of light propagation, as depicted in Fig. 2.13b. Connection between input intensity (\( I_{in} \)) and reflected intensity (\( I'_{bn} \)) is established with transfer matrix method for non-interference film.
2.4 Optical model of transparent photodetector

The change of the order of subsystems has no influence on the transmission 
\[ \left( \eta_{\text{glass}} \right| r_{\text{air,glass}} \right) \right|^2 \cdot \left( \eta_{\text{glass}} \right| r_{\text{glass,air}} \right) \right|^2 \), and Eq. (2.126) remains valid. However, to obtain the quantum efficiency, it is necessary to take into account that part of the light enters the detector subsystem from the glass substrate. The quantum efficiency is given by:

\[ QE = T_{\text{air},i} \left( 1 - \exp(-\alpha_i d_i) + R_{i,n} \exp(-\alpha_i d_i) - R_{i,n} \exp(-2\alpha_i d_i) + \frac{4\kappa_i}{n_i} \sqrt{R_{i,n}} \exp(-\alpha_i d_i) \sin \left( \frac{2\pi}{\lambda} n_i d_i \right) \cos \left( \frac{2\pi}{\lambda} n_i d_i - \arg(r_{i,n}) \right) \right) + \frac{T_{\text{det}} T_{\text{glass},i}}{1 - R_{\text{int}} R_{\text{det}}} \left( 1 - \exp(-\alpha_i d_i) + R_{i,p} \exp(-\alpha_i d_i) - R_{i,p} \exp(-2\alpha_i d_i) + \frac{4\kappa_i}{n_i} \sqrt{R_{i,p}} \exp(-\alpha_i d_i) \sin \left( \frac{2\pi}{\lambda} n_i d_i \right) \cos \left( \frac{2\pi}{\lambda} n_i d_i - \arg(r_{i,p}) \right) \right) \]  

(2.128)

where \( R_{i,n} \) is the reflectivity of layers behind the i-layer, and \( T_{\text{air},i} \) is the transmission from air into the i-layer. Transfer matrix elements \( r_{i,n} \), \( r_{i,p} \) (Fig. 2.13b) are used to determine these values. Equation (2.128) states that the quantum efficiency of the transparent photodetector in this case is the sum of two contribution, which correspond to forward and backward propagating light.

### 2.4.1 Results

The quantum efficiency can be experimentally determined by measuring the photocurrent of a detector for a specific wavelength of the incoming light. By using the light source with known power, the quantum efficiency is calculated according to Eq. (2.4).
2. Transparent photodetector

The quantum efficiency of the transparent photodetector has been measured from the glass side and back ZnO electrode side [19, 35]. The transmission of the transparent photodetector is measured with an UV-VIS-NIR spectrometer that covers ultraviolet, visible and infrared part of the electromagnetic spectrum. Figure 2.14 depicts experimentally measured and simulated properties of the transparent photodetector.

Experimentally measured quantum efficiencies and transmission of the transparent photodetector are shown in Fig. 2.14a. The measured results for the quantum efficiency are adapted from literature [19]. When light enters from the glass side of the transparent photodetector, the quantum efficiency exhibits maximum of 38% for a wavelength of 452 nm. For shorter wavelengths, the quantum efficiency is low due to the absorption in the front ZnO antireflection coating and the n-layer. For longer wavelengths, the quantum efficiency drops due to the small absorption coefficient of the amorphous silicon (Fig. 2.2a). The quantum efficiency is close to zero for wavelengths longer than 700 nm. When light enters from the side of back ZnO electrode, the maximum of the quantum efficiency (27.5%) is achieved for a wavelength of 500 nm. For shorter wavelengths, the quantum efficiency is low due to the absorption in the back ZnO electrode and p-layer. Since the p-layer is thicker than the n-layer [19], the rising edge of the quantum efficiency is slightly shifted towards longer wavelengths compared to the case when light enters from the glass side. Again, the quantum efficiency is almost zero for wavelengths longer than 700 nm. The transparent photodetector shows almost no transmission for wavelengths shorter than 350 nm. The transmission increases for wavelengths longer than 400 nm and achieves maximum value of 86.6% for a wavelength of 645 nm, which is close to the aimed wavelength of 633 nm [19].

Simulated quantum efficiencies and transmission of the transparent photodetector are shown in Fig. 2.14b. As described in Sec. 2.3.2, the optimal optical thickness of the antireflection coatings should be an odd multiple of quarter of a wavelength, while optical thickness of the p-i-n diode should be an integer multiple of half of the wavelength. However, in order to achieve a good agreement with experimental results, simulations are conducted for a thickness of the front ZnO electrode of 260 nm (optical
2.4 Optical model of transparent photodetector

thickness \sim 2.93 \cdot \lambda/4), n-layer thickness of 18 nm (\sim 0.2 \cdot \lambda/2), i-layer thickness of 37 nm (\sim 0.48 \cdot \lambda/2), p-layer thickness of 34 nm (\sim 0.32 \cdot \lambda/2) and back ZnO electrode thickness of 210 nm (\sim 2.4 \cdot \lambda/4). The simulated quantum efficiency, when the light enters from the glass side, exhibits maximum of 38.5 % for a wavelength of 425 nm. For the back ZnO side, the maximum quantum efficiency (30.6 %) is achieved for a wavelength of 485 nm. Same as for the experimental measurements, the rising edge of the glass side quantum efficiency is shifted toward shorter wavelengths, which is influenced by the smaller thickness of the n-layer. Irrespectively of the side from which light is entering the transparent detector, the simulated quantum efficiency is zero for wavelengths longer than 730 nm. The simulated transmission exhibits maximum of 82.6 % for a wavelength of 670 nm. The simulated quantum efficiencies are shifted by 15-25 nm toward shorter wavelengths compared to the measured results. On the other hand, the simulated transmission is shifted towards longer wavelengths by 25 nm. However, the developed optical models are able to match and predict the behavior of the transparent photodetector. Therefore, the measured and simulated optical properties of the transparent photodetector shown in Fig. 2.14 exhibit relatively good agreement.
2. Transparent photodetector
Chapter 3

Transparent photodetector - applications

Most common applications of transparent photodetectors are in the fields of interferometry and Fourier transform spectroscopy. Interferometers are optical devices used for high precision length measurements or positioning of objects with nanometer accuracy. Interferometer systems require a light source of a known wavelength (laser or laser diode) and a directional sensitivity, which is realized by combining two transparent photodetectors and a phase shifter [36]. Fourier transform spectrometers are used to determine the spectrum of an unknown light source using Fourier transform. These devices require a single transparent photodetector and a precise distance measurement [18, 20, 34, 35, 37, 59]. A transparent photodetector is used to realize optical spectrometers and interferometers based on the sampling of a standing wave and Fabry-Perot resonator [17, 18, 20, 21, 34–37, 59, 60]. For the standing wave based devices, a plane mirror is used to form a standing wave, while the Fabry-Perot resonator is formed between a low reflectivity reflector and a transparent photodetector. The transparent photodetector is used to record the interference pattern of the light source as a function of the optical path difference. The spectrum of the light source is obtained by Fourier transform of the recorded interferogram [14, 15, 61].

The focus of this chapter is on the experimental realization and modeling of the standing wave and transparent Fabry-Perot spectrometer. The fundamentals of the Fourier transform spectroscopy are introduced at the beginning of this chapter. Experimental results are presented and described with different optical models of spectrometers. Furthermore, optical models for an incoherent light source are also presented. Parts of this chapter are adapted from previously published papers [21, 60].

3.1 Fourier Transform Spectroscopy

The classical setup of a Fourier transform spectrometer is based on a Michelson spectrometer, which is schematically depicted in Fig. 3.1. The input beam from the light source is divided by a beam splitter. One resulting beam gets reflected by a fixed mirror and another by a moving mirror. The position of the moving mirror is denoted with $z_m$. For the position of the moving mirror $z_m = 0$, the resulting beams travel the same distance. By changing the position of the moving mirror, a path difference equal to twice the position of the moving mirror ($\Delta L = 2z_m$) is introduced. After reflection, the beams are recombined at the beam splitter where they interfere. Consequently,
the output beam is the result of interference between the waves propagating in the same direction.

Assuming that the interfering beams are monochromatic plane waves, the intensity of the output beam in a Michelson spectrometer is given by Eq. (2.68). Since the intensity of interfering waves is equal \( I_1 = I_2 = I_0 \), Eq. (2.68) can be rewritten:

\[
I = I_0 \left( 1 + \cos \left( \frac{2\pi}{\lambda_0} Z \right) \right) = I_0 \left( 1 + \cos \left( 2\pi f_0 Z \right) \right)
\]  

(3.1)

where \( Z \) denotes the optical path difference \( (Z = \Delta L = 2z_m) \), \( \lambda_0 \) is the wavelength of the monochromatic plane wave, and \( f_0 \) is the corresponding frequency \( (f_0 = 1/\lambda_0) \).

Equation (3.1) can be generalized for a light source with a wide band spectrum \( (B(f)) \), which is shown in Fig. 3.2. Based on Fig. 3.2, the interference equation for the monochromatic section \( (df) \) around certain frequency \( (f) \) of the wide band spectrum is given by:

\[
dI(Z, f) = B(f) \, df \left( 1 + \cos \left( 2\pi f Z \right) \right)
\]

(3.2)

In order to obtain the total signal for the complete spectrum, integration is required:

\[
I(Z) = \bar{I}(Z) + \tilde{I}(Z) = \int_{0}^{\infty} B(f) \, df + \int_{0}^{\infty} B(f) \cos \left( 2\pi f Z \right) \, df
\]

(3.3)

where \( I(Z) \) is called the interference record [14, 15]. The alternating component (AC) of the interference record \( (\tilde{I}(Z)) \) is called the interferogram [14, 15].

The relationship between the interferogram and wide band spectrum can be simplified by constructing the symmetrical spectrum \( (B_e(f)) \) [14, 15]:

\[
B_e(f) = \frac{1}{2} (B(f) + B(-f))
\]

(3.4)

The interferogram is now given by:

\[
\tilde{I}(Z) = \int_{-\infty}^{\infty} B_e(f) \cos \left( 2\pi f Z \right) \, df = \int_{-\infty}^{\infty} B_e(f) \exp \left( i2\pi f Z \right) \, df
\]

(3.5)
Equation (3.5) states that the interferogram is the inverse Fourier transform of the spectrum. Consequently, the interferogram and spectrum of the light source form a Fourier transform pair [14, 15]. By switching to wave vector \( k = 2\pi f \), the relationship between the spectrum and interferogram can be written as:

\[
B_e(k) = \int_{-\infty}^{\infty} \tilde{I}(Z) \exp(-ikZ) \, dZ \tag{3.6}
\]

\[
\tilde{I}(Z) = \frac{1}{2\pi} \int_{-\infty}^{\infty} B_e(k) \exp(ikZ) \, dk \tag{3.7}
\]

Equation (3.6) shows that the spectrum of the light source can be obtained by Fourier transform of the measured interferogram. This is the fundamental principle of Fourier transform spectroscopy.

The main advantages of the Fourier transform spectrometers are multiplexing and high throughput [14, 15]. Multiplexing is the ability of spectrometers to simultaneously detect multiple wavelengths, while throughput represents efficiency of spectrometers to gather light. High throughput is necessary for spectrometers to rapidly gather spectral information of the light source. Consequently, Fourier transform spectrometers are useful for measuring weak and broad spectra [14, 15], which is needed for spectral imaging in many domains [3–9].

**Influence of coherence.** The interferogram of the monochromatic and coherent light source (Fig. 3.3a) for Michelson spectrometer can be derived from Eq. (3.1):

\[
\tilde{I} = I_0 \cos(2k_0 z_m)
\]

where the position of the mirror \((z_m)\) is used instead of the optical path difference \((Z)\). The corresponding Fourier transform is given by [61, 62]:

\[
\mathcal{F}\{\tilde{I}\} = \pi I_0 \delta(k' + 2k_0) + \pi I_0 \delta(k' - 2k_0) \tag{3.9}
\]

where \(\delta(k')\) is Dirac delta function. The spectrum of the monochromatic light source is properly obtained by replacing the wave vector \(k'\) by \(2k\):

\[
\mathcal{F}\{\tilde{I}\} = \pi \frac{I_0}{2} \delta(k + k_0) + \pi \frac{I_0}{2} \delta(k - k_0) \tag{3.10}
\]
Figure 3.3: (a) Interferogram of the monochromatic and coherent light source, and (b) corresponding spectrum.

where scaling properties of Dirac delta function are used [61, 62]. Equation (3.10) states that the spectrum of the monochromatic light source is represented by a Dirac impulse which is shifted to the wave vector ($k_0$) of the monochromatic light (Fig. 3.3b). The interferogram and the spectrum of the monochromatic light source are shown in Fig. 3.3.

By taking into account that the intensities of the interfering waves in the Michelson spectrometer are equal to half of the input wave, the interferogram of the monochromatic and partially coherent light source can be derived from Eqs. (2.98) and (2.100):

$$I = I_0 \cos (2k_0 z_m) \cdot \exp \left( -\frac{2\pi z_m^2}{L_c^2} \right)$$ (3.11)

Equation (3.11) shows that the interferogram of the partially coherent monochromatic light is a product of a cosine and Gaussian function (Fig. 3.4a). To determine the Fourier transform of the product of different functions, convolution theorem is applied [61, 62]. Consequently, the Fourier transform of the interferogram is given by:

$$\mathcal{F} \{\tilde{I}\} = \frac{\sqrt{2}}{2} L_c I_0 \frac{1}{2} \exp \left( -\frac{L_c^2 (k + k_0)^2}{2\pi} \right) + \frac{\sqrt{2}}{2} L_c I_0 \frac{1}{2} \exp \left( -\frac{L_c^2 (k - k_0)^2}{2\pi} \right)$$ (3.12)

The spectrum of the partially coherent monochromatic light source is represented by Gaussian function which is shifted to the wave vector of the light source ($k_0$). Full width at half maximum (FWHM) of the spectrum is given by [61]:

$$FWHM = 2\sqrt{2\pi \ln 2} \frac{L_c}{L_c}$$ (3.13)

Equation (3.13) reveals the connection between the width of the spectrum and the coherence length. A light source with a wide band spectrum exhibits small coherence length and vice versa. For significantly large values of the coherence length, the spectrum can be approximated by Dirac function as given by Eq. (3.10). The interferogram and the spectrum of the partially coherent monochromatic light source are shown in Fig. 3.4.
3.1 Fourier Transform Spectroscopy

Figure 3.4: (a) Interferogram of monochromatic and partially coherent light source, and (b) corresponding spectrum.

Influence of finite recording region and discrete sampling. The spectrum of the monochromatic light source given by Eq. (3.10) is valid only for the case of continuous Fourier transform, which requires infinite and continuous spatial recording of the interferogram. In practice, the interferogram is recorded only in a finite region and sampled at discrete points.

To describe the interferogram recorded in the finite region (Fig. 3.5a), the rectangular function can be used [14, 15, 61, 62]. Assuming that the finite recording region is symmetrical to the position of the mirror \( z_m = 0 \), the interferogram equation of the monochromatic and coherent plane wave (Eq. (3.8)) becomes:

\[
\tilde{I} = I_0 \cos (2k_0 z_m) \cdot \text{rect} \left[ \frac{z_m}{L_R} \right] \quad (3.14)
\]

where \( L_R \) is the length of the recording region. Since the interferogram is the product of two functions, the convolution theorem is used to determine the spectrum. For the finite recording region, the spectrum of the monochromatic and coherent light source is given by:

\[
\mathcal{F} \left\{ \tilde{I} \right\} = L_R I_0 \frac{1}{2} \text{sinc} \left( (k + k_0) L_R \right) + L_R I_0 \frac{1}{2} \text{sinc} \left( (k - k_0) L_R \right) \quad (3.15)
\]

where \( \text{sinc} (k) = \frac{\sin (k)}{k} \). Equation (3.15) shows that, due to the finite interferogram recording, the spectrum of the monochromatic and coherent light source is described by the sinc function shifted to the wave vector of the light (Fig. 3.5b). The interferogram and the spectrum of the monochromatic light source for finite recording are shown in Fig. 3.5. The finite recording of the interferogram defines theoretical resolution and broadening of spectral lines. The theoretical resolution is given by the FWHM [14, 15]:

\[
\text{FWHM} \approx 1.207 \frac{\pi}{L_R} \quad (3.16)
\]

The broadening of spectral lines is defined by the first zero of the sinc function (Fig. 3.5b):

\[
\Delta k = \frac{2\pi}{L_R} \quad (3.17)
\]
For a wide band light source, the broadening of spectral lines has the largest influence on the minimum value of the wave vector ($k_{\text{min}}$). In order to reduce the influence of the broadening on the measured spectrum, it is necessary to have a sufficiently large recording region so that $k_{\text{min}} \gg \Delta k$. Consequently, the condition for the length of the recording region is given by:

$$L_R \gg \lambda_{\text{max}}$$

(3.18)

where $\lambda_{\text{max}}$ is the wavelength that corresponds to the minimum wave vector ($k_{\text{min}}$).

The sampled interferogram (Fig. 3.6a) can be described by the Dirac comb function [61, 62]. The interferogram equation (Eq. (3.8)) is given by:

$$\tilde{I} = I_0 \cos (2k_0z_m) \cdot \sum_{n=-\infty}^{+\infty} \delta (z_m - n \cdot \Delta z)$$

(3.19)

where $\Delta z$ is the distance (period) between sampling points. By applying the convolution theorem, the spectrum is obtained:

$$\mathcal{F}\{\tilde{I}\} = \frac{\pi}{\Delta z} \frac{I_0}{2} \sum_{n=-\infty}^{+\infty} \delta \left( k + k_0 - n \cdot \frac{\pi}{\Delta z} \right) + \frac{\pi}{\Delta z} \frac{I_0}{2} \sum_{m=-\infty}^{+\infty} \delta \left( k - k_0 - m \cdot \frac{\pi}{\Delta z} \right)$$

(3.20)

The spectrum of the monochromatic light source, instead of two Dirac functions at positive and negative wave vector values (Fig. 3.3b), is represented with two Dirac comb functions with period $\frac{\pi}{\Delta z}$ (Fig. 3.6b). The sampled interferogram and corresponding spectrum are shown in Fig. 3.6.

The Dirac comb functions at positive ($k_0$) and negative wave vector ($-k_0$) value are infinite sums which overlap with each other (Fig. 3.3b). Depending on the overlap, the measured spectrum can be a correct or incorrect representation of the light source spectrum. Figure 3.6b represents the case when the measured spectrum is not the correct representation of the monochromatic light source. In this case, the sampling period is too large and the overlap occurs within the region of interest ($0, k_0$). Since there are two Dirac functions, one at the correct value of $k_0$ and one at the wrong
value of $-k_0 + \frac{\pi}{\Delta z}$, the measured spectrum represents the spectrum of a light source that emits two wavelengths.

To determine the critical sampling period it is necessary to analyze the case of the wide band spectrum represented in Fig. 3.7. Due to sampling, the measured spectrum of a wide band light source that occupies wave vector region $(-k_{max}, k_{max})$ is a periodically recurring function with a period same as for the monochromatic case. In order to eliminate the overlap between recurring elements, the period has to be larger than the spectrum band ($\pi \Delta z \geq 2k_{max}$). Consequently, the critical sampling interval ($\Delta z_c$) is given by:

$$\Delta z_c = \frac{\lambda_{min}}{4}$$  \hspace{1cm} (3.21)

where $\lambda_{min}$ is the wavelength that corresponds to the maximum wave vector ($k_{max}$). Equation (3.21) represent Nyquist criterion for sampling of the interferogram. If the sampling period is larger than the critical value ($\Delta z > \Delta z_c$), an aliasing effect is present, and the spectrum is distorted due to overlap of recurring elements [14, 15]. If the sampling period is much smaller than the critical value ($\Delta z \ll \Delta z_c$), oversampling occurs since more data than necessary is collected. To properly record the interferogram of a light source, it is necessary to record it for a sufficiently large
region (Eq. (3.18)), with a sufficiently small sampling period \((\Delta z \leq \Delta z_c)\).

### 3.2 Standing wave spectrometer

A standing wave is an interference pattern that is formed in front of a reflective surface such as a plane mirror. The mirror reflects the light, which leads to an interference between the input and reflected beam, and a creation of a standing wave. Unlike the Michelson spectrometer, the interferogram of the standing wave spectrometer is the result of the interference of waves that propagate in opposite direction. In the case of monochromatic plane waves, the standing wave pattern is described by the interference equation (Eq. (2.68)). The phase difference between the input and reflected wave is a sum of the path difference between the waves and the phase change introduced by the mirror. Assuming that the mirror is able to reflect the incoming light perfectly, the phase difference is given by:

\[
\varphi = 2k_0 z_m + \pi
\]

(3.22)

where \(z_m\) is the distance between the observation position and the mirror, and \(\pi\) is the phase change due to the mirror reflectivity. The distance between the transparent detector and the mirror is defined by the starting position \((z_0 \geq 0)\) and the length of the recording region \((z_m \in (z_0, z_0 + L_R))\) (Fig. 3.8). Due to the perfect reflectivity of the mirror, the intensity of the reflected wave is equal to the input wave \((I_1 = I_2 = I_0)\), and the equation of the standing wave pattern is given by:

\[
I = 2I_0 (1 - \cos (2k_0 z_m)) = 4I_0 \sin^2 (k_0 z_m)
\]

(3.23)

From Eq. (3.23), the interferogram of the standing wave pattern can be expressed as:

\[
\tilde{I} = -2I_0 \cos (2k_0 z_m)
\]

(3.24)

The interferogram of the standing wave spectrometer is different from the interferogram of the Michelson spectrometer (Eq. (3.8)) only by a constant factor of
3.2 Standing wave spectrometer

Therefore, the properties of the Fourier transform spectroscopy derived for the Michelson spectrometer are also valid in this case.

To record the interferogram, it is necessary to introduce a transparent photodetector into the standing wave and change the distance between the detector (observation position) and mirror \( z_m \). Due to the configuration of the standing wave spectrometer, the negative values of \( z_m \) can not be achieved, and the interferogram is recorded only for positive values. The setup of the standing wave spectrometer is presented in Fig. 3.8.

3.2.1 Basic operating principles

The interferogram given by Eq. (3.24) is independent of the transparent detector properties. In practice, the transparent photodetector has a significant influence on the standing wave pattern and the recorded interferogram. By analyzing the influence of the transparent photodetector on the recorded interferogram, the optimal dimensions of the transparent photodetector and instrumental function of the standing wave spectrometer can be determined.

The instrumental function of the spectrometer represents its output in the wave vector domain under monochromatic illumination [14, 15]. In other words, the instrumental function of the spectrometer is the Fourier transform of the recorded interferogram. The instrumental function determines the influence of the spectrometer on the light source spectrum. For a wide band light source, the output of the spectrometer is a convolution of the light source spectrum and instrumental function.

Basic operating principles of the standing wave spectrometer are demonstrated by representing the transparent photodetector only by the i-layer of p-i-n photodiode. The i-layer is described by the complex refractive index \( N_i = \eta_i - i\kappa_i \) and thickness \( d_i \). The recorded interferogram and instrumental function are derived for the ideal and realistic model of the standing wave spectrometer.

**Ideal model.** For the ideal model it is assumed that the standing wave pattern is not affected by the transparent photodetector. In other words, the transparent photodetector exhibits no reflectivity at its surfaces and absorbs negligible amount of light. In reality, this is possible only if the i-layer material has optical properties of air with small absorption coefficient. Nevertheless, the optical properties of the a-Si:H are used to describe the i-layer. Furthermore, the plane mirror is represented by the perfect reflector. By introducing the transparent photodetector into the standing wave pattern, only a small part of the standing wave pattern is located within the photodetector (Fig. 3.9).

Figure 3.9 schematically represents basic operating principles of an ideal standing wave spectrometer. The dashed lines are used to mark the mirror and standing wave pattern for the first position of the mirror \( z_{m1} \), while the full lines are used for the second position \( z_{m2} \). For the position \( z_{m1} \), the transparent photodetector absorbs a certain part of the standing wave pattern (dashed line within the photodetector) and generates a photocurrent. By moving the mirror to the position \( z_{m2} \), a different part of the standing wave pattern is located within the photodetector (full line within the photodetector), and a different photocurrent is generated. To determine the photocurrent of the transparent photodetector, it is necessary to derive the expression for the intensity of the standing wave within the detector.
3. Transparent photodetector - applications

For the ideal transparent photodetector, the electric field within the i-layer for the incident monochromatic plane wave with a given amplitude \(E_0\) and wave vector \(k_0 = \frac{2\pi}{\lambda_0}\) can be represented as:

\[
E(z) = E_0 \exp(-ik_i z) + E_0 \exp(-i(2k_0 z_m + \pi)) \exp(-ik_i (2d_i - z))
\]  
(3.25)

where \(z \in (0, d_i)\) is the position within the i-layer, and \(k_i = k_0 \cdot N_i\) is the wave vector in the i-layer. By replacing Eq. (3.25) into Eq. (2.46), the light intensity within the i-layer as a function of the mirror position is obtained:

\[
I_i(z) = I_0 \eta_i \left( \exp(-\alpha_i z) + \exp(-\alpha_i (2d_i - z)) - 2 \exp(-\alpha_i d_i) \cos(2k_0 \eta_i (d_i - z) + 2k_0 z_m) \right)
\]  
(3.26)

where \(\alpha_i\) is the absorption coefficient of the i-layer material. Equation (3.26) is analogous to Eq. (3.23), and describes the forward and backward propagating wave, and interference component. The generated photocurrent is obtained by replacing Eq. (3.26) into Eq. (2.8) and solving the integral in Eq. (2.11):

\[
I_{ph}(z_m) = -\frac{qA}{hc} I_0 \lambda_0 \eta_i \left( 1 - \exp(-2\alpha_i d_i) - \frac{4\kappa_i}{\eta_i} \exp(-\alpha_i d_i) \sin \left( \frac{2\pi}{\lambda_0} \eta_i d_i \right) \cos \left( 2k_0 \left( z_m + \frac{\eta_i d_i}{2} \right) \right) \right)
\]  
(3.27)

where \(A\) is the active area of the transparent photodetector. Equation (3.27) represents the generated photocurrent as a function of the distance between the transparent detector and the mirror. The generated photocurrent carries information about the standing wave pattern influenced by the properties of the transparent photodetector. By analyzing the generated photocurrent, the operating range and instrumental function of the standing wave spectrometer, and the optimal dimensions of the transparent photodetector can be obtained.

Figure 3.9: Basic operating principles of an ideal standing wave spectrometer.
To determine the optimal dimensions of the transparent photodetector and operating range of the standing wave spectrometer, quantities such as sensitivity, visibility and selectivity can be used [18, 59]. The sensitivity represents the signal of the transparent photodetector generated by the direct component (DC) of the standing wave pattern [59]. In this study, the sensitivity is defined by an absolute value of the DC photocurrent ($I_{ph}$):

$$SEN = |I_{ph}|$$

(3.28)

The sensitivity for the ideal model of the standing wave spectrometer is obtained by replacing Eq. (3.27) into Eq. (3.28) and removing the interference element:

$$SEN = \frac{qA}{hc} I \lambda \eta_i (1 - \exp (-2\alpha_i d_i))$$

(3.29)

where $I$ is the input light intensity for a specific wavelength ($\lambda$).

The visibility represents the signal generated by the transparent photodetector due to the interferogram of the standing wave [18]. The visibility is usually defined as the difference between the minimum and maximum amplitude of the AC photocurrent [18]. In this study, the root mean square (RMS) amplitude of the AC photocurrent is used to define the visibility:

$$VIS = (\tilde{I}_{ph})^{RMS}$$

(3.30)

By removing the DC photocurrent from Eq. (3.27), the visibility of the ideal standing wave spectrometer is given by:

$$VIS = 2\sqrt{2} \frac{qA}{hc} I \lambda \kappa_i \eta_i \exp (-\alpha_i d_i) \left| \sin \left( \frac{2\pi \lambda \eta_i d_i}{\lambda} \right) \right|$$

(3.31)

As stated in Sec. 3.1, the spectral information of the light source is determined by the interferogram. Therefore, the AC photocurrent represents the signal, while the DC component can be treated as a noise [59]. For the Fourier transform spectrometers, a quantity of signal-to-noise ratio can be represented by the selectivity [59]. The selectivity is defined by the ratio of the visibility and sensitivity [59]. In this study, the selectivity is given as the ratio between RMS amplitude of the AC photocurrent and the absolute value of the DC photocurrent:

$$SEL = \frac{(\tilde{I}_{ph})^{RMS}}{|I_{ph}|}$$

(3.32)

The selectivity for the ideal standing wave spectrometer is given by:

$$SEL = \frac{2\sqrt{2} \kappa_i \exp (-\alpha_i d_i) \left| \sin \left( \frac{2\pi \eta_i d_i}{\lambda} \right) \right|}{\eta_i (1 - \exp (-2\alpha_i d_i))}$$

(3.33)

To determine the sensitivity, visibility and selectivity, it is assumed that the intensity of light is 1 W/m$^2$ for all the wavelengths and that the area of photodetector is 1 cm$^2$. These properties of the ideal standing wave spectrometer are then calculated from Eqs. (3.29), (3.31) and (3.33).
Figure 3.10: Properties of the standing wave spectrometer obtained by the ideal model. (a) Sensitivity, (b) visibility and (c) selectivity of the ideal standing wave spectrometer.

Figure 3.10 depicts the sensitivity, visibility and selectivity of the ideal standing wave spectrometer for wavelengths of 300 nm, 500 nm and 700 nm as a function of the i-layer thickness. The sensitivity is shown in Fig. 3.10a. For small thicknesses of the i-layer, the sensitivity increases with increasing i-layer thickness. After a certain critical thickness, all the light gets absorbed in the i-layer, and the sensitivity remains constant with further increase of the i-layer thickness. The critical thickness of the i-layer at which the sensitivity remains constant depends on the optical properties of the i-layer material. For a wavelength of 300 nm, the critical thickness is around 50 nm. On the other hand, the critical thickness for a wavelength of 500 nm is close to 400 nm.

Figure 3.10b depicts the visibility of the ideal standing wave spectrometer. According to Eq. (3.31), the visibility achieves peak values ($|\sin \left( \frac{2\pi}{\lambda} \eta_i d_i \right)| = 1$) when the optical thickness of the i-layer is equal to an odd integer multiple of quarter of the wavelength. Due to the absorption in the i-layer, the maximum value is achieved for the first peak ($\eta_i d_i = \lambda/4$). The minimum of the visibility ($|\sin \left( \frac{2\pi}{\lambda} \eta_i d_i \right)| = 0$) is achieved when the optical thickness is equal to an integer multiple of half of the wavelength. After the critical thickness of the i-layer is reached, the visibility becomes zero since all the light is absorbed in the i-layer, and a standing wave can not be formed. The selectivity of the standing wave spectrometer according to the ideal model is shown in Fig. 3.10c. The selectivity is high for small thicknesses of the i-layer and becomes zero after a
3.2 Standing wave spectrometer

critical thickness of the i-layer is reached. In order to achieve good selectivity for the complete absorption range of a-Si (300-800 nm), the optimal thickness of the standing wave spectrometer should be less than 20 nm. However, for such a thin i-layer, the visibility of wavelengths longer than 750 nm is close to zero, and the output signal is negligible. By increasing the i-layer thickness, the visibility of longer wavelengths is slightly improved, but at the same time the visibility of shorter wavelengths drops. If the i-layer thickness is 37 nm, the visibility is larger than zero for all wavelengths of interest excluding the wavelength of 361 nm, for which the minimum visibility condition is satisfied. Consequently, the operating range in this case is 300-360 nm and 362-800 nm.

The instrumental function of the ideal standing wave spectrometer can be determined by obtaining the Fourier transform of the AC photocurrent. According to Eq. (3.27), the AC photocurrent is given by:

\[ I_{ph}^{AC} (z_m) = 4 \frac{qA}{hc} I_0 \lambda_0 \kappa_i \exp (-\alpha_i d_i) \sin \left( \frac{2\pi}{\lambda_0} \eta_i d_i \right) \cos \left( 2k_0 \left( z_m + \frac{\eta_i d_i}{2} \right) \right) \] (3.34)

In order to determine the Fourier transform, the finite recording region (Eq. (3.35)) and discrete sampling (Eq. (3.19)) of the AC photocurrent have to be taken into account (Sec. 3.1). Therefore, the interferogram recorded by the ideal standing wave spectrometer is given by:

\[ \tilde{I} = 4 \frac{qA}{hc} I_0 \lambda_0 \kappa_i \exp (-\alpha_i d_i) \sin \left( \frac{2\pi}{\lambda_0} \eta_i d_i \right) \cos \left( 2k_0 \left( z_m + \frac{\eta_i d_i}{2} \right) \right) \cdot \right\] 

\[ \cdot \text{rect} \left[ \frac{z_m - L_R/2 - z_0}{L_R} \right] \cdot \sum_{n=-\infty}^{+\infty} \delta (z_m - z_0 - n \cdot \Delta z) \] (3.35)

The arguments of the rectangular and Dirac comb function in Eq. (3.35) are different than in Eqs. (3.14) and (3.19) to account for the fact that the interferogram is sampled only for the positive mirror positions. Assuming that the sampling period (\( \Delta z \)) is smaller than the critical value given by Eq. (3.21), the instrumental function of the ideal standing wave spectrometer is given by the Fourier transform of Eq. (3.35) for positive wave vectors and replica \( m = 0 \):

\[ \mathcal{F} \left\{ \tilde{I} \right\} = 2 \frac{qA}{hc} I_0 \lambda_0 \kappa_i N_{sp} \exp (-\alpha_i d_i) \sin \left( \frac{2\pi}{\lambda_0} \eta_i d_i \right) \exp \left( i \frac{2\pi}{\lambda_0} \eta_i d_i \right) \cdot \exp (-i (k - k_0) (L_R + 2z_0)) \cdot \text{sinc} \left( (k - k_0) L_R \right) \] (3.36)

where \( N_{sp} \) represents the number of sampling points (\( N_{sp} = L_R/\Delta z \)). The instrumental function of the ideal standing wave spectrometer is a sinc function which is shifted to the wave vector of the monochromatic light. The amplitude of the sinc function carries information of the light source intensity. The resolution of the spectrometer is defined by the FWHM of the sinc function (Eq. (3.16)). To evaluate the instrumental function and spectrum of the light, only the absolute value of the Fourier transform is used [18, 35, 59, 63, 64]. The absolute value of the instrumental function is given by:

\[ \left| \mathcal{F} \left\{ \tilde{I} \right\} \right| = 2 \frac{qA}{hc} I_0 \lambda_0 \kappa_i N_{sp} \exp (-\alpha_i d_i) \left| \sin \left( \frac{2\pi}{\lambda_0} \eta_i d_i \right) \right| \cdot \text{sinc} \left( (k - k_0) L_R \right) \] (3.37)
In practice, the instrumental function is determined by the discrete Fourier transform (DFT) of the sampled interferogram. Fast Fourier transform (FFT) is an algorithm used to calculate DFT. The simulated instrumental functions of the ideal standing wave spectrometer are presented in Fig. 3.11.

Figure 3.11a shows the instrumental functions computed for a wavelength of 500 nm using FFT algorithm and Eq. (3.37) and assuming the same recording length and number of sampling points. An excellent agreement between these approaches is observed. Consequently, Eq. (3.37) can be used to evaluate properties of instrumental functions which are calculated by the FFT algorithm. Figure 3.11b depicts the instrumental function for wavelengths of 500 nm and 700 nm. Instrumental functions are calculated by applying the FFT algorithm to the AC photocurrent (Eq. (3.34)) assuming that the light intensity is same for both wavelengths. The length of the recording region and number of sampling points are used as parameters. The presented results for wavelength of 500 nm show that the amplitude of the sinc function increases if the number of sampling points is increased. For wavelength of 700 nm, the sinc function exhibits smaller amplitude than for wavelength of 500 nm with same number of sampling points. Therefore, the amplitude of the instrumental function depends on the number of sampling points and the spectrometer visibility. If the calculated spectrum is normalized to the number of sampling points and visibility of the spectrometer for a specific wavelength, the amplitude of the sinc function depends only on the light intensity for that specific wavelength. The length of the recording region influences only the resolution (FWHM) of the spectrometer. In the wave vector domain, the resolution is independent of the wave vector, and it is determined by the recording length (Eq. (3.16)). However, for the wavelength domain, the resolution depends on the wavelength as shown in Fig. 3.11b. The FWHM in the wavelength domain is given by:

\[
FWHM \approx \frac{1.207 \cdot \lambda^2}{2L_R}
\]  

(3.38)

Equation (3.38) is derived by replacing a derivative of Eq. (2.35) into Eq. (3.16).
According to Eq. (3.38), for the same recording length, the resolution for wavelength of 500 nm is better than for wavelength of 700 nm as shown in Fig. 3.11b.

**Realistic model.** For the realistic model, the propagation of the light through the i-layer is modeled using transfer matrix method for interference films (Sec. 2.3.2). Again, a-Si:H is used to describe the i-layer material, while the plane mirror is represented by the optical properties of silver [65]. In this model, the transparent photodetector influences the standing wave pattern when it is introduced into it. Nevertheless, by changing the distance between the transparent detector and mirror, the standing wave pattern moves within the detector (Fig. 3.12b). Consequently, the photocurrent is modulated by the mirror movement. The operating principles of the realistic standing wave spectrometer are shown in Fig. 3.12.

Figure 3.12a depicts the elements of interference transfer matrix method used for realistic modeling of the standing wave spectrometer. As shown by the model presented in Sec. 2.3.2, the transmission ($\tilde{t}_{\text{air},i}$) and reflection coefficient ($\tilde{r}_{\text{i,air}}$) depend on the distance between the transparent detector and mirror ($\tilde{t}_{\text{air},i} = \tilde{t}_{\text{air},i}(z_m)$ and $\tilde{r}_{\text{i,air}} = \tilde{r}_{\text{i,air}}(z_m)$). By moving the mirror from $z_m1$ to $z_m2$, both the amplitude and phase of these coefficients are changing. Similar to the Fabry-Perot resonator (Sec. 2.3.2), the transmission and reflection coefficients are periodic functions of the mirror position. The electric field within the i-layer is given by Eq. (2.95) where number indexing should be replaced by layer names. To evaluate the profile of the standing wave located in the i-layer, the electric field intensity can be used. Figure 3.12b shows the profile of the standing wave for distances $z_m1$ and $z_m2$ between the detector and mirror. The profile of the standing wave within the i-layer changes with the position of the mirror. The intensity of the light within the i-layer is given by Eq. (2.96) where the layer name ($i$) should be used instead of the number index ($j$). Furthermore, the transmission and reflectivity into the i-layer, and the argument of the reflection coefficient are now functions of the mirror position ($T_{0,j} = T_{\text{air},i}(z_m) = \eta_i |\tilde{t}_{\text{air},i}(z_m)|^2$, $R_{j,j+1} = R_{i,\text{air}}(z_m) = |\tilde{r}_{i,\text{air}}(z_m)|^2$ and $\arg(\tilde{r}_{j,j+1}) = \arg(\tilde{r}_{i,\text{air}}(z_m))$). The photocurrent is obtained by replacing the light intensity within the i-layer into Eq. (2.8) and

---

**Figure 3.12:** (a) Transfer matrix elements and (b) basic operating principles for the realistic model of the standing wave spectrometer.
solving the integral in Eq. (2.11):

\[
I_{ph}(z_m) = -\frac{qA}{h\varepsilon} I_0 \lambda_0 T_{air,i}(z_m) \left( 1 - \exp(-\alpha_i d_i) + R_{t,air}(z_m) \exp(-\alpha_i d_i) - R_{t,air}(z_m) \exp(-2\alpha_i d_i) + 4 \kappa_i \eta_i \sqrt{R_{t,air}(z_m)} \exp(-\alpha_i d_i) \cdot \sin\left(\frac{2\pi}{\lambda_0} \eta_i d_i\right) \cos\left(\frac{2\pi}{\lambda_0} \eta_i d_i - \arg(\tilde{r}_{t,air}(z_m))\right) \right)
\]

Equation (3.39) shows that the generated photocurrent for the realistic standing wave spectrometer depends on the amount of light that reaches the i-layer (determined by the transmission into the i-layer) and the absorption within the i-layer (determined by the expression in brackets).

To determine the properties of the realistic standing wave spectrometer, the AC and DC photocurrent can be calculated numerically from Eq. (3.39). Alternatively, the DC photocurrent can also be obtained by optical modeling. Based on the examples shown in Sec. 2.3.2, the DC photocurrent can be calculated from the layer system where the air gap between the i-layer and the mirror is represented as a non-coherent layer. Consequently, the interference and non-interference transfer matrix methods are combined as shown in Sec. 2.4. The expression for the DC photocurrent is analogous to the quantum efficiency for the back side model of the transparent photodetector (Eq. (2.128)) and depends on the light intensities that come from the front and the back side of the i-layer. In this case, the DC photocurrent has to be deducted from the total current given by Eq. (3.39) to get the AC photocurrent. After determining the AC and DC photocurrent, the sensitivity, visibility and selectivity of the realistic standing wave spectrometer can be obtained from Eqs. (3.28), (3.30) and (3.32), respectively.

The sensitivity, visibility and selectivity for wavelengths of 300 nm, 500 nm and 700 nm as a function of the i-layer thickness are shown in Fig. 3.13. Same as for the ideal model, the sensitivity increases with increasing i-layer thickness, which can be observed in Fig. 3.13a. The sensitivity exhibits fringes due to the interference effects in the i-layer. When the thickness of the i-layer is larger than the critical thickness, the sensitivity remains constant, and the interference fringes disappear. The critical thickness of the i-layer again represents the thickness when all the light that enters the i-layer gets absorbed, and the standing wave pattern disappears. Therefore, the critical thickness for different wavelengths is the same as for the ideal model. The visibility is shown in Fig. 3.13b. Due to the fact that transmission \(T_{air,i}(z_m)\) and reflectivity into the i-layer \(R_{t,air}(z_m)\) are periodic functions of the mirror position, the conditions for the minimum \(|\sin\left(\frac{2\pi}{\lambda_0} \eta_i d_i\right) = 0\) and maximum \(|\sin\left(\frac{2\pi}{\lambda_0} \eta_i d_i\right) = 1\) of the visibility defined for the ideal model are not valid in this case. The visibility for the realistic model is always higher than zero until the critical thickness of the i-layer is reached. The sensitivity and visibility are lower than for the ideal model due to the reflectivity of the transparent detector surface. Figure 3.13c depicts the selectivity according to the realistic model of the standing wave spectrometer. The selectivity is larger than zero if the i-layer thickness is smaller than the critical value. For the thickness of the i-layer smaller than 20 nm, good selectivity can be achieved for all wavelengths that are absorbed by a-Si:H. However, the visibility of longer wavelengths is then small. By increasing the i-layer thickness, the visibility of the
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Figure 3.13: Properties of the standing wave spectrometer obtained by the interference transfer matrix method. (a) Sensitivity, (b) visibility and (c) selectivity of the realistic standing wave spectrometer for wavelengths of 300 nm, 500 nm, and 700 nm, assuming light intensity of 1 W/m², and the area of detector of 1 cm².

longer wavelengths (>700 nm) is improved, but at the same time the visibility of the shorter wavelengths (<400 nm) drops. For an i-layer thickness of 37 nm, the operating range is defined by the visibility and covers all wavelengths in range of 300-800 nm.

The instrumental function is obtained by applying the FFT algorithm to the recorded interferogram (AC photocurrent). The AC photocurrent is calculated numerically from Eq. (3.39) for wavelengths of 500 nm and 700 nm, assuming that the light intensity is same for both wavelengths. To exclude the influence of the visibility, the AC photocurrent is normalized by the visibility for the specific wavelength. Normalized AC photocurrents are shown in Fig. 3.14. Figure 3.14a depicts the AC photocurrent for the wavelength of 500 nm. The AC photocurrent is a periodic function of the mirror movement with the same angular frequency as for the ideal model (2k₀). However, the AC photocurrent significantly deviates from the ideal cosine response (Eq. (3.34)). The deviation is caused by the Fabry-Perot resonator, which is formed between the i-layer and the mirror. Similar behavior is observed for the AC photocurrent for the wavelength of 700 nm, which is shown in Fig. 3.14b. The deviations for the wavelengths of 500 nm and 700 nm are different, since the absorption of the i-layer depends on the Fabry-Perot oscillations. Due to the deviation from the cosine function, the AC photocurrent can be represented by a Fourier series [14, 15, 62].
The components of the Fourier series are cosine functions with angular frequencies equal to an integer multiple of \(2k_0\). The amplitude of each component depends on its correlation with the AC photocurrent. Consequently, the instrumental function is a sum of sinc functions shifted to the wave vector of the monochromatic light source \((k_0)\) and corresponding higher order harmonics (integer multiples of the wave vector).

Figure 3.15 depicts the instrumental functions in wave vector and wavelength domain according to the realistic model of the standing wave spectrometer. The instrumental functions are obtained from the calculated interferograms (Fig. 3.14) for a recording length of 10 \(\mu\)m. In the wave vector domain (Fig. 3.15a), the instrumental functions are represented by sinc functions shifted to the wave vector of the monochromatic light and corresponding integer multiples. Same as for the ideal model of the standing wave spectrometer, the resolution in the wave vector domain is independent of the wave vector, and it is given by the Eq. (3.16).

In the wavelength domain (Fig. 3.15a), the instrumental function is represented by sinc functions shifted to the wavelength of the light source and an integer fractions of the wavelength. For the wavelength range of interest (300-800 nm), besides the peaks at wavelengths of 500 nm and 700 nm, an additional peak at 350 nm is also present. The appearance of the higher order harmonics defines the free spectral range in which the light spectrum is determined correctly. Therefore, the operating range of the standing wave spectrometer depends not only on the visibility of the spectrometer, but also on the free spectral range of the Fabry-Perot resonator that is formed between the transparent detector and the mirror \([60]\).

The upper limit of the operating range \(\lambda_{OR}^{max}\) is defined by the upper limit of the visibility, while the lower operating limit depends on the free spectral range. Since the upper limit of the visibility is 800 nm for an i-layer thickness of 37 nm, the free spectral range defines 400 nm as the lower operating limit. Due to the broadening of spectral lines (Eq. (3.17)), the lower operating limit also depends on the recording length. Therefore, the lower limit of the operating range \((\lambda_{OR}^{min})\) is given by:

\[
\lambda_{OR}^{min} = \frac{\lambda_{OR}^{max}}{2} + \left(\frac{\lambda_{OR}^{max}}{2}\right)^2 \frac{8L_R}{2}
\]

\[(3.40)\]
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Based on Eq. (3.40), for the recording length of 10 $\mu$m, the operating range of the standing wave spectrometer is roughly 408-800 nm. The resolution in the wavelength domain is the same as for the ideal model (Eq. (3.38)). To properly obtain the spectrum, the instrumental functions shown in Fig. 3.15 are normalized to the number of sampling points. However, the peaks of the sinc functions at 500 nm and 700 nm do not have the same value, although it is assumed that the light intensity is the same for both wavelengths. Due to Fabry-Perot oscillations, the peak of the sinc function carries information of the light source intensity multiplied by the Fourier series coefficients. Since the Fourier series coefficients are different for different wavelengths in this case, the determined spectrum is inaccurate. To improve accuracy of the standing wave spectrometer, it is necessary to suppress higher order harmonics and reduce the deviation from the cosine function for all wavelengths of interest [20]. In practice, this is achieved by coating the transparent photodetector with antireflection coatings [19, 20, 35, 59, 64]. The antireflection coatings reduce the influence of the Fabry-Perot resonator, and the AC photocurrent exhibits quasi-cosine behavior. Consequently, the Fourier coefficient for the first harmonic is closer to unity, and the peak of the sinc function depends only on the light source intensity.

3.2.2 Experimental realization and results

A standing wave spectrometer has been realized by placing a transparent photodetector in front of a silver mirror. To change the distance between the transparent detector and the mirror, the mirror is mounted on a piezo microactuator. The movement of the microactuator and the mirror is controlled by a function generator. The movement of the mirror can be described by cosine oscillations. The frequency of the oscillation has been 100 Hz, while the difference between the minimum and maximum mirror position (recording length) is set to 6.6 $\mu$m. To experimentally determine the instrumental function of the standing wave spectrometer, a helium-neon (HeNe) laser emitting at a wavelength of 633 nm is used as a light source. The photocurrent generated by the transparent photodetector is amplified using a low noise current amplifier and sampled.
Figure 3.16: Measured (a) AC photocurrent and (b) mirror movement as a function of the time. (c) Recorded interferogram.

by a digital oscilloscope with a sampling interval of 4 μs. Since the AC photocurrent represents the recorded interferogram, the DC photocurrent is filtered out. Due to the oscillatory and non-linear mirror movement, the AC photocurrent is recorded only during half of the oscillation as a non-linear function of time (Fig. 3.16a). By recording the mirror movement as a function of time (Fig. 3.16b), the “photocurrent versus time” can be shown as “photocurrent versus mirror movement” (Fig. 3.16c). Figure 3.16 depicts the measured AC photocurrent and mirror movement as a function of time, and the recorded interferogram (AC photocurrent) as a function of the mirror movement.

The experimentally realized standing wave spectrometer is modeled using the interference transfer matrix method, since the coherence length of the laser light source is significantly larger than the thicknesses of all layers that compose the spectrometer. The elements of interference transfer matrix method are shown in Fig. 3.17. Equation (3.39) is used to calculate the total generated photocurrent, where $R_{i,\text{air}}(z_m)$ and $\arg (\tilde{r}_{i,\text{air}}(z_m))$ should be replaced by $R_{i,p}(z_m) = |\tilde{r}_{i,p}(z_m)|^2$ and $\arg (\tilde{r}_{i,p}(z_m))$, respectively. The DC photocurrent is also obtained by optical modeling, where the air gap between the transparent photodetector and the mirror is treated as a non-coherent layer. The AC photocurrent is obtained by deducting the DC photocurrent from the total photocurrent.

Figure 3.18 depicts the simulated and measured AC photocurrents (recorded interferograms) for the experimentally realized standing wave spectrometer. The amplitudes of the AC photocurrents are normalized to one for easier comparison. The ideal case described by a cosine function is shown as a reference. Relatively good
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Figure 3.17: Elements of interference transfer matrix method for the experimentally realized standing wave spectrometer.

Figure 3.18: Measured and simulated AC photocurrent for a wavelength of 633 nm.

agreement between the measured and simulated results is observed. The measured and simulated AC photocurrents exhibit quasi-cosine behavior with small deviation from the ideal cosine function. The quasi-cosine behavior is influenced by the antireflection properties of the ZnO electrodes. The measured AC photocurrent exhibits better agreement with the cosine function than the simulated current. This could be influenced by a misalignment between the transparent photodetector and the mirror in the experiment, which reduces the Fabry-Perot effect [18]. The instrumental function of the experimentally realized standing wave spectrometer is obtained by applying FFT algorithm to the measured and simulated interferogram.

The simulated and measured instrumental functions of the experimentally realized standing wave spectrometer are shown in Fig. 3.19. The instrumental functions are normalized by the number of sampling points. Figure 3.19a depicts the instrumental functions in the wave vector domain. The instrumental functions are the sum of sinc functions placed at the wave vector of the light source and corresponding higher order harmonics. Figure 3.19b shows the instrumental functions in the wavelength domain, where additional peak appears at a wavelength of 316 nm. The peak value of the sinc
function at wavelength of 633 nm is slightly higher for the measured case, since the measured interferogram is closer to the ideal cosine response. Amplitudes of higher order harmonics are suppressed due to the antireflection coatings, and the accuracy of the determined spectrum is improved. The higher order harmonics influence the operating range of the standing wave spectrometer. To define the upper limit of the experimentally realized standing wave spectrometer, the measured quantum efficiency of the transparent photodetector (Fig. 2.14a) is used. By multiplying the measured quantum efficiency with the wavelength of light, the upper limit of the operating range is determined to be 750 nm. The lower limit of the operating range is calculated from Eq. (3.40). Therefore, for the recording length of 6.6 \( \mu \)m, the operating range of the experimentally realized standing wave spectrometer is 385-750 nm. The resolution of the spectrometer in the wave vector and wavelength domain is again given by Eqs. (3.16) and (3.38), respectively.

### 3.3 Transparent Fabry-Perot spectrometer

The main component of a Fabry-Perot spectrometer is the resonator that is formed between two reflective surfaces (Fig. 3.20a). The basic principles of the Fabry-Perot resonator are demonstrated in Sec. 2.3.2. By changing the distance between the reflectors, the transmission through the resonator (Eq. (2.122)) is modulated (Fig. 2.9a). Assuming that the reflectors are low reflectivity surfaces (\( R \leq 2 - \sqrt{3} \)) without absorption (\( R = 1 - T \)), which is valid for glass sheet reflectors, Eq. (2.122) can be simplified, and the intensity of the transmitted light is given by:

\[
I = I_0 \left( 1 - \frac{2R}{(1-R)^2} + \frac{2R}{(1-R)^2} \cos(2k_0z_m) \right)
\]  

where the resonator thickness is denoted by \( z_m \). The resonator thickness is defined by the starting position (\( z_0 \geq 0 \)) and the length of the recording region (\( z_m \in (z_0, z_0 + L_R) \)). From Eq. (3.41), the interferogram of the Fabry-Perot resonator can

![Figure 3.19: Measured and simulated instrumental function of the experimentally realized standing wave spectrometer as a function of the (a) wave vector and (b) wavelength.](image)
be expressed by:

\[
\tilde{I} = \frac{2R}{(1-R)^2}I_0 \cos(2k_0z_m)
\] (3.42)

Since the interferogram of the Fabry-Perot resonator is different from the Michelson spectrometer interferogram (Eq. (3.8)) by a constant factor, the properties of the Fourier transform spectroscopy described in Sec. 3.1 are also valid in this case. Due to the similar configuration as for the standing wave spectrometer, the interferogram of the Fabry-Perot resonator can be recorded only for positive values of the resonator thickness.

The Fabry-Perot spectrometer is typically realized by placing a photodetector behind the Fabry-Perot resonator. To create a transparent Fabry-Perot spectrometer, the stationary reflector is replaced by a transparent photodetector (Fig. 3.20b). A Fabry-Perot resonator and transparent Fabry-Perot spectrometer are schematically depicted in Fig. 3.20.

### 3.3.1 Operating principles

The interferogram of the Fabry-Perot resonator (Eq. (3.42)) depends on the properties of its reflectors. Therefore, the recorded interferogram of the transparent Fabry-Perot spectrometer is influenced by the properties of the resonator and transparent photodetector. By analyzing the recorded interferogram, the optimal dimensions of the transparent photodetector and instrumental function of the transparent Fabry-Perot spectrometer can be obtained.

To determine the recorded interferogram, a simplified model of the Fabry-Perot spectrometer is analyzed. In this model, it is assumed that the transmission through the Fabry-Perot resonator is described by Eq. (2.122). The light that passes through the resonator enters the transparent photodetector, where part of it gets absorbed. The multiple reflections between the Fabry-Perot resonator and transparent detector are neglected. Furthermore, the transparent detector is represented only by the i-layer of the p-i-n photodiode. The propagation of light through the i-layer is described by
the interference transfer matrix method. The optical properties of a-Si:H are used to describe the i-layer.

The basic operating principles of the transparent Fabry-Perot spectrometer and transfer matrix elements are shown in Fig. 3.21. The dashed lines are used to mark the electric field intensity for the first position of the moving reflector \((z_{m1})\), while the full lines are used for the second position \((z_{m2})\). By changing the position of the moving reflector from \(z_{m1}\) to \(z_{m2}\), the intensity of the light that enters the transparent detector is modulated. The photocurrent generated in the i-layer is calculated from Eq. (3.39), where \(I_0\) should be multiplied by Eq. (2.122), and \(\arg(\tilde{t}_{air,1})\) should be replaced by \(\arg(r_{i,air})\). Also, it has to be noted that \(T_{air,i} = \eta_i |\tilde{t}_{air,i}|^2\) and \(R_{i,air} = |r_{i,air}|^2\) are independent of the position of the moving reflector. Therefore, the absorption of the i-layer is independent on the Fabry-Perot oscillations, unlike for the standing wave spectrometer. The DC photocurrent is also obtained from Eq. (3.39), where corresponding transfer matrix elements are replaced with elements from Fig. 3.21, and \(I_0\) is multiplied by Eq. (2.123). The AC photocurrent is determined as a difference between the total and DC photocurrent. The AC and DC photocurrents are used to calculate the sensitivity (Eq. (3.28)), visibility (Eq. (3.30)) and selectivity (Eq. (3.32)) of the Fabry-Perot spectrometer.

The sensitivity, visibility and selectivity for wavelengths of 300 nm, 500 nm and 700 nm as a function of the i-layer thickness are shown in Fig. 3.22. Again, the light intensity is 1 W/m², and the area of photodetector is 1 cm². For the Fabry-Perot spectrometer, the resonator thickness determines the amount of light that reaches the i-layer. At the same time, the absorption of the light in the i-layer is independent on the resonator thickness. Therefore, the visibility and sensitivity exhibit same trends for a specific wavelength, which is depicted in Fig. 3.22a. With increasing thickness of the i-layer, the sensitivity and visibility also increase. After reaching the critical thickness of the i-layer, the sensitivity and visibility are constant, and no light is transmitted through the Fabry-Perot spectrometer. Therefore, the optimal thickness of the transparent photodetector depends on the trade-off between the strength of the generated signal and transmission of the spectrometer. The selectivity of the Fabry-Perot spectrometer is independent of the i-layer thickness and equal for all
3.3 Transparent Fabry-Perot spectrometer

Figure 3.22: (a) Sensitivity/visibility for wavelengths of 300 nm, 500 nm and 700 nm, and (b) selectivity of the transparent Fabry-Perot spectrometer.

Figure 3.23: AC photocurrent as a function of the resonator thickness for wavelengths of (a) 500 nm and (b) 700 nm.

wavelengths (Fig. 3.22b). The selectivity of the Fabry-Perot spectrometer is influenced by the reflectivity of the resonator reflectors. Since the reflectors have small reflectivity, the selectivity is significantly smaller than for the standing wave spectrometer (Fig. 3.13c). The selectivity of the Fabry-Perot spectrometer can be improved by increasing the reflectivity of the reflectors, but at the same time the interferogram will deviate more from the ideal cosine function [54, 56]. The operating range of the Fabry-Perot spectrometer is influenced by the visibility. For an i-layer thickness of 37 nm, the visibility covers all wavelengths in range of 300-750 nm.

Figure 3.23 depicts the AC photocurrents (recorded interferograms) of the Fabry-Perot spectrometer for wavelengths of 500 nm and 700 nm. The AC photocurrents are normalized by the visibility for the specific wavelength. The AC photocurrent for a wavelength of 500 nm is shown in Fig. 3.23a. The AC photocurrent is a periodic function of the resonator thickness that slightly deviates from the cosine function. The deviation is caused by the properties of the Fabry-Perot resonator. The AC photocurrent for a wavelength of 700 nm is shown in Fig. 3.23b. For wavelength of 700 nm, the AC photocurrent exhibits larger period than for 500 nm. Since the
properties of the Fabry-Perot resonator are independent of the wavelength, deviations of the AC photocurrent from the cosine function are equal for both wavelengths.

The instrumental functions of the Fabry-Perot spectrometer in the wave vector and wavelength domain for input wavelengths of 500 nm and 700 nm are shown in Fig. 3.24. The instrumental functions are normalized to the number of sampling points and obtained for a recording length of 10 \( \mu \text{m} \). The instrumental function of the transparent Fabry-Perot spectrometer is also represented by a sinc function. Therefore, the resolutions of the Fabry-Perot spectrometer in the wave vector (Fig. 3.24a) and wavelength domain (Fig. 3.24b) are given by Eqs. (3.16) and (3.38), respectively. The amplitude of the sinc functions for wavelengths of 500 nm and 700 nm are equal, unlike the standing wave spectrometer. This is influenced by the fact that the properties of the Fabry-Perot resonator are wavelength independent. Therefore, the Fabry-Perot spectrometer determines the spectrum with the same accuracy as the Michelson spectrometer.

Higher order harmonics are present in the instrumental function of the transparent Fabry-Perot spectrometer. Consequently, the operating range of the Fabry-Perot spectrometer should be obtained from Eq. (3.40), where the upper limit is determined by the visibility. In such a case, the operating range of the Fabry-Perot spectrometer for a recording length of 10 \( \mu \text{m} \) is 385-750 nm. However, for a Fabry-Perot spectrometer with low reflectivity reflectors, it can be assumed that the suppression of the higher order harmonics is sufficiently large. Therefore, the operating range of the transparent Fabry-Perot spectrometer is determined only by the visibility. For an i-layer thickness of 37 nm, the operating range of the transparent Fabry-Perot spectrometer is 300-750 nm.

### 3.3.2 Experimental realization and results

The transparent Fabry-Perot spectrometer is realized by placing a glass sheet in front of the transparent photodetector. To change the thickness of the Fabry-Perot resonator, the glass sheet is mounted on the piezo microactuator. The recording length has been set to 6.25 \( \mu \text{m} \). The remaining experimental settings and procedures are the
3.3 Transparent Fabry-Perot spectrometer

Figure 3.25: Elements of interference transfer matrix method for the experimentally realized transparent Fabry-Perot spectrometer.

same as for the experimentally realized standing wave spectrometer (Sec. 3.2.2).

Due to the large coherence length of the laser light source, the interference transfer matrix method is used to model the experimentally realized Fabry-Perot spectrometer. The transfer matrix elements are shown in Fig. 3.25. Equation (3.39) is used to calculate the total photocurrent, where $R_{i,\text{air}}(z_m)$ and $\arg(\tilde{r}_{i,\text{air}}(z_m))$ should be replaced by $R_{i,p} = |\tilde{r}_{i,p}|^2$ and $\arg(\tilde{r}_{i,p})$, respectively. By describing the air gap of the Fabry-Perot resonator as a non-coherent film, the DC photocurrent is calculated. By deducting the DC photocurrent from the total photocurrent, the recorded interferogram is obtained.

The measured and simulated AC photocurrents of the experimentally realized transparent Fabry-Perot spectrometer are shown in Fig. 3.26. To allow for easy comparison, the amplitudes of the AC photocurrents are normalized to one. The ideal case of the cosine function is shown as a reference. Good agreement between the ideal, measured and simulated AC photocurrent is observed. The agreement is influenced by the fact that the transparent photodetector is optimized for a wavelength of 633 nm [19]. The measured AC photocurrent exhibits variations in the amplitude due to noise. The FFT algorithm is used to calculate the instrumental functions.

Figure 3.27 depicts the instrumental functions of the experimentally realized transparent Fabry-Perot spectrometer which are obtained by measurement and modeling. The number of the sampling points is used to normalize their peak value. The instrumental functions in the wave vector domain are shown in Fig. 3.27a, while Fig. 3.27b depicts the wavelength domain. From Fig. 3.27 it can be observed that higher order harmonics are not present, which is influenced by the optimized transmission of the transparent photodetector. Consequently, the free spectral range can be neglected when determining the operating range. The operating range of experimentally realized spectrometer is roughly 310-750 nm, which is determined from the measured quantum efficiency (Fig. 2.14a) multiplied by the wavelength of light. The resolution of the experimentally realized Fabry-Perot spectrometer is given by Eqs. (3.16) and (3.38).
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Figure 3.26: Measured and simulated AC photocurrent for a wavelength of 633 nm.

Figure 3.27: Measured and simulated instrumental function of experimentally realized Fabry-Perot spectrometer in the (a) wave vector and (b) wavelength domain.

3.4 Partially coherent light

The developed models of the experimentally realized standing wave and Fabry-Perot spectrometer are accurate under the assumption that the incoming light is coherent monochromatic plane wave. This is valid in the case of the laser light source. However, for light sources with shorter coherence lengths, the developed models are insufficient, and separate optical models have to be created.

To develop the partially coherent models, it is assumed that the thick glass layers are non-coherent (Sec. 2.4). The degree of correlation (Eq. (2.100)) depends on the distance between the transparent photodetector and the mirror (standing wave spectrometer) or reflector (Fabry-Perot spectrometer). To describe this dependence, it is necessary to combine the interference and non-interference transfer matrix method as demonstrated in Sec. 2.3.2. The partially coherent Fabry-Perot resonator is already shown in Sec. 2.3.2. Therefore, for the partially coherent model of the Fabry-Perot spectrometer, the results from Sec. 2.3.2 are used. The partially coherent model of the standing wave spectrometer is developed using analogous approach.
3.4 Partially coherent light

**Fabry-Perot spectrometer - partially coherent model.** A schematic representation of the partially coherent Fabry-Perot spectrometer is shown in Fig. 3.28. The interference transfer matrix method is used to determine the transmission and the reflectivity of the air/glass interface, and the reflectivity of the detector stack. The transmission \( T_{PC}^{res} \) and reflectivity \( R_{PC}^{res} \) of the partially coherent Fabry-Perot resonator (Sec. 2.3.2) are used to describe the light propagation through the partially coherent system. The transmission of the partially coherent Fabry-Perot resonator is given by Eq. (2.125), and for the reflectivity an analogous equation is valid. The non-interference transfer matrix method is then used to determine the connection between the input light intensity \( I_{in} \) and the light intensity that reaches the transparent photodetector \( I'_{in} \). The transmission factor \( I'_{in}/I_{in} \) depends on the transmission and reflectivity of the partially coherent system, the transmission and reflectivity of the interface \( T_{int}, R_{int} \), and the reflectivity of the detector stack \( R_{det} \). The generated photocurrent is calculated from Eq. (3.39), where \( I_{0} \) is replaced by \( I_{in} \) multiplied by the transmission factor obtained from the non-interference transfer matrix method. Furthermore, the transmission and reflectivity into the i-layer are determined from the interference transfer matrix elements shown in Fig. 2.12b.

The sensitivity (Eq. (3.28)), visibility (Eq. (3.30)) and selectivity (Eq. (3.32)) of the transparent Fabry-Perot spectrometer are obtained from the generated photocurrent, again assuming that the light intensity is 1 W/m² and the area of photodetector is 1 cm². The DC photocurrent is calculated assuming small coherence length of the light and large thickness of the Fabry-Perot resonator \( z_{m} \gg L_{c} \). To determine the AC photocurrent, it is assumed that the coherence length is significantly larger than the resonator thickness \( L_{c} \gg z_{m} \), and then the DC photocurrent is subtracted from the total photocurrent. The results are shown in Fig. 3.29.

Figure 3.29a depicts the sensitivity and visibility according to the partially coherent model of the Fabry-Perot spectrometer. Unlike the model presented in Sec. 3.3.1, the visibility and sensitivity are not equal for all wavelengths. The light reflected by
the detector stack interacts with the Fabry-Perot resonator and modulates the light intensity that reaches the i-layer. For the model presented in Sec. 3.3.1, this interaction is neglected. Based on the visibility, the transparent Fabry-Perot spectrometer covers wavelengths in range 310-750 nm. The selectivity of the partially coherent Fabry-Perot spectrometer is shown in Fig. 3.29b. The selectivity is small and determined by the reflectivity of the reflectors. The observed modulation of the selectivity is influenced by the reflectivity of the detector stack.

Figure 3.30 depicts the AC photocurrents of the Fabry-Perot spectrometer for the partially coherent light assuming coherence length of 5 \( \mu \)m and 20 \( \mu \)m. The photocurrents are normalized by the visibility for the specific wavelength. Figure 3.30a shows the AC photocurrent for the input wavelength of 500 nm. The photocurrent amplitude depends on the coherence length and the thickness of the resonator. Figure 3.30b depicts the results for the input wavelength of 700 nm. The period of the AC photocurrent is increased, while the influence of the coherence length is the same as for the previous case. From the AC photocurrents, the instrumental functions are
3.4 Partially coherent light

Figure 3.31: Instrumental functions of the partially coherent light for coherence length of (a) 5 \( \mu \text{m} \) and (b) 20 \( \mu \text{m} \), using different recording settings for the Fabry-Perot spectrometer.

determined assuming different recording settings (Fig. 3.31).

Figure 3.31a depicts the instrumental functions for wavelengths of 500 nm (red curve) and 700 nm (blue curve) calculated for a coherence length of 5 \( \mu \text{m} \) with recording length of 5 \( \mu \text{m} \) and minimum resonator thickness of zero. The curves are normalized to the number of sampling points, and they can be described by Gaussian functions shifted to the wavelength of the light and corresponding higher order harmonics. The peak values of instrumental functions are independent of wavelength, and the Fabry-Perot spectrometer accurately determines the spectrum in this case. Furthermore, it can be observed that the higher order harmonics can be neglected.

Based on Eqs. (3.13) and (2.35), the resolution in wavelength domain is given by:

$$ FWHM = \frac{\lambda^2}{L_C} \sqrt{\frac{2 \ln 2}{\pi}} \quad (3.43) $$

According to Eq. (3.43), the FWHM for wavelengths of 500 nm and 700 nm with coherence length of 5 \( \mu \text{m} \) are 33 nm and 65 nm, respectively. However, FWHM of the instrumental functions are roughly 60 nm (red curve) and 117 nm (blue curve) (Fig. 3.31a). In order to properly determine the resolution, it is necessary to take into account the finite recording region. Consequently, FWHM has to be calculated as the sum of Eqs. (3.38) and (3.43). By using this approach, the resolutions are calculated to be 63 nm (\( \lambda = 500 \text{ nm} \)) and 124 nm (\( \lambda = 700 \text{ nm} \)), which is in a good agreement with the observed values. Therefore, the resolution of the partially coherent light depends on the coherence length and recording settings.

To further investigate the influence of recording settings on the resolution, the instrumental functions are calculated for a wavelength of 500 nm using recording length of 10 \( \mu \text{m} \) with minimum resonator thickness of zero (dashed green curve) and recording length of 5 \( \mu \text{m} \) with a starting resonator thickness of 2 \( \mu \text{m} \) (black curve). For easier comparison, the curves are normalized to have the same peak value. By keeping the minimum resonator thickness constant (\( z_0 = 0 \ \mu \text{m} \)) and increasing the recording length, the resolution of the spectrometer remains the same. This is influenced by the fact that in this case the AC photocurrent becomes zero after a certain thickness of the
Fabry-Perot resonator. Therefore, it is necessary to introduce the effective recording length as the region in which the interferogram can be recorded.

The effective recording length is represented by the distance between the minimum resonator thickness and resonator thickness at which the AC photocurrent becomes zero. The maximum resonator thickness is determined by the coherence length, while the minimum resonator thickness is determined by the spectrometer setup. By increasing the minimum thickness of the resonator ($z_0 = 2 \, \mu m$), the effective recording length is reduced and the FWHM of the spectrum is increased (Fig. 3.31a). Compared to the Michelson spectrometer, the largest effective recording length of the Fabry-Perot spectrometer is two times smaller since negative path difference cannot be achieved in a linear setup.

Figure 3.31b depicts the instrumental functions for wavelengths of 500 nm (red curve) and 700 nm (blue curve) calculated for a coherence length of 20 $\mu m$ with recording length of 20 $\mu m$ and minimum resonator thickness of zero. The FWHM are now 16 nm and 30 nm for the wavelengths of 500 nm and 700 nm, respectively. The observed values are in a good agreement with the theoretical values of FWHM (Eq. (3.38) + Eq. (3.43)), which are 16 nm and 31 nm.

Figure 3.31b also depicts the instrumental functions for a wavelength of 700 nm, where the recording length is 5 $\mu m$ with minimum resonator thickness of zero (green curve) and 15 $\mu m$ (black curve). When the coherence length is much larger than the recording length, the instrumental function is a convolution of a sinc and Gaussian function. For the minimum resonator thickness of 0 $\mu m$, the sinc function dominates since the change of the AC photocurrent is small in this region (Fig. 3.30). When the minimum resonator thickness is large ($z_0 = 15 \, \mu m$), the Gaussian function dominates since the change of the amplitude of the AC photocurrent is larger.

To properly determine the spectrum of the partially coherent light, the complete interferogram has to be recorded. Therefore, the minimum resonator thickness should be as small as possible, while the recording length should be equal or larger than the coherence length of the light. For practical applications of the Fabry-Perot spectrometer, a recording length of 20 $\mu m$ and minimum resonator thickness of 0 $\mu m$ are necessary to properly determine the spectrum of the wide band light sources [56]. If the coherence length of the light is smaller than 20 $\mu m$, the FFT has to be applied only to sampled points where the AC photocurrent is larger than zero, and the effective recording length should be included into calculations.

In general, the operating range of the Fabry-Perot spectrometer for the wide band light depends on the effective recording length, the visibility of the spectrometer and the appearance of the second order harmonics. However, for practical realization with low reflectivity glass reflectors, it can be assumed that the suppression of the second order harmonic is sufficiently large (Fig. 3.31). In such case, the operating range is determined only by the visibility and covers wavelengths within the range 310-750 nm.

Standing wave spectrometer - partially coherent model. The schematic representation of the partially coherent standing wave spectrometer is shown in Fig. 3.32. To determine the reflectivity ($R_{det}^{PC}$) and generated photocurrent ($I_{ph}^{PC}$) of the partially coherent system, it is necessary to use the approach demonstrated in Sec. 2.3.2. In the first step, the partially coherent system is modeled only by interference transfer matrix method to obtain the complete reflectivity and generated photocurrent. In the next step, the air gap between the transparent photodetector and the silver
3.4 Partially coherent light

Figure 3.32: Schematic representation of a partially coherent standing wave spectrometer and elements of transfer matrix method for non-interference films.

mirror is assumed to be a non-coherent layer. By combining the interference and non-interference transfer matrix methods, the direct components of the reflectivity and the photocurrent are obtained. By applying Eq. (2.125) to the obtained complete and direct components, the reflectivity and photocurrent of the partially coherent system are determined. In the last step, the transmission ($T_{int}$) and reflectivity ($R_{int}$) of the interface are used to calculate the ratio between the input light intensity ($I_{in}$) and the light intensity that reaches the transparent photodetector ($I'_{in}$). The total photocurrent generated in the i-layer is given by:

$$I_{ph} = \frac{T_{int}}{1 - R_{int} \cdot R_{det}^{PC}} \cdot I_{PC}^{ph}$$  \hspace{1cm} (3.44)

From Eq. (3.44) the sensitivity, visibility and selectivity are calculated (Fig. 3.33).

Figure 3.33a depicts the sensitivity and visibility of the standing wave spectrometer for the partially coherent light source. Due to the absorption in the front ZnO layer and n-layer, the sensitivity is zero for wavelengths shorter than 310 nm same as for the Fabry-Perot spectrometer. For longer wavelengths, the sensitivity of the standing wave spectrometer is higher than for the Fabry-Perot spectrometer since the light is passing through the transparent detector before and after being reflected by the silver mirror. The visibility of the standing wave spectrometer is zero for wavelengths shorter than 380 nm. To form a standing wave, the light has to pass through the transparent photodetector and then back into the i-layer after being reflected by the silver mirror. The appearance of the two peaks for the visibility can be contributed to the reflectivity of the transparent photodetector from the back ZnO side. The visibility of the standing wave spectrometer covers wavelengths in range 380-800 nm. Compared to the Fabry-Perot spectrometer, the visibility is higher since the silver mirror reflects most of the light, and intensity of the backward wave is comparable to the input wave. The selectivity of the standing wave spectrometer increases for longer wavelengths as shown in Fig. 3.33b. The standing wave spectrometer exhibits higher selectivity than the
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Figure 3.33: (a) Sensitivity, visibility and (b) selectivity of the standing wave spectrometer for the partially coherent light.

Figure 3.34: The recorded interferograms of the standing wave spectrometer for wavelengths of (a) 500 nm and (b) 700 nm assuming coherence length of 10 μm.

Fabry-Perot spectrometer.

The simulated interferograms of the standing wave spectrometer for a light source with a coherence length of 10 μm are shown in Fig. 3.34. The simulated AC photocurrents are normalized to exclude the influence of the visibility for a specific wavelength. Figure 3.34a depicts the recorded interferogram for a wavelength of 500 nm. The AC photocurrent is a periodic function of the mirror movement with decreasing amplitude due to the coherence length of the light. Similar behavior is observed for a wavelength of 700 nm. The AC photocurrent for the wavelength of 700 nm is shown in Fig. 3.34b. Due to the antireflection properties of ZnO electrodes, the deviations between the AC photocurrent for wavelength of 500 nm and 700 nm are reduced compared to the realistic model of the standing wave spectrometer (Fig. 3.14). However, compared to the Fabry-Perot spectrometer, the AC photocurrent deviates more from the ideal cosine function. From the simulated interferograms, the instrumental functions are calculated (Fig. 3.35).

Figure 3.35 depicts the spectrum curves for wavelengths of 500 nm (red curve) and 700 nm (blue curve) assuming a coherence length of 10 μm. The recording length
3.5 Discussion and summary

In this chapter, the applications of a transparent photodetector in Fourier transform spectroscopy are presented. The transparent photodetector is used to experimentally realize a standing wave and Fabry-Perot spectrometer. To create different optical models of the realized spectrometers, the interference and non-interference transfer matrix methods are implemented. The developed models are used to determine the spectrometer properties such as the operating range, accuracy and strength of the generated signal.

The standing wave spectrometer utilizes a transparent photodetector to sample a standing wave that is formed in front of a silver mirror. On the other hand, the Fabry-Perot spectrometer utilizes the properties of a Fabry-Perot resonator to create interference pattern, while the transparent photodetector records the pattern and enables operation in transmission. Although the basic operating principles of the

is 10 µm and minimum resonator thickness is 0 µm. The instrumental functions are normalized to the number of sampling points. The maximum values are not equal, since the antireflection coatings are not perfect. However, the accuracy of the spectrometer is improved compared to the case without antireflection coatings (Fig. 3.15). The FWHM are 29 nm and 58 nm for the wavelengths of 500 nm and 700 nm, respectively. The theoretical values of FWHM (Eq. (3.38) + Eq. (3.43)) are 32 nm and 62 nm, which is in a good agreement with observed values. The higher order harmonics can also be observed in Fig. 3.35.

For the standing wave spectrometer the suppression of the second order harmonic is not sufficient. Therefore, the free spectral range has to be taken into account when determining the operating range. The upper limit of the operating range is defined by the visibility. The lower limit is defined by the second order harmonic and broadening of spectral lines due to the finite recording region (Eq. (3.40)). For sunlight, the maximum effective recording length (\( z_0 = 0 \) µm) is almost 1 µm [56]. The operating range of the standing wave spectrometer in such a case is 480-800 nm.

Figure 3.35: Instrumental function of the standing wave spectrometer for the light source with coherence length of 10 µm assuming effective recording length of 10 µm.

![Instrumental function diagram](image-url)
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standing wave and Fabry-Perot spectrometer are different, their performances and properties are comparable.

The recorded interferograms of the standing wave and Fabry-Perot spectrometer deviate from the ideal cosine response of the Michelson spectrometer. The deviations are influenced by the properties of the Fabry-Perot resonator. For the standing wave spectrometer, the Fabry-Perot resonator is formed between the transparent photodetector and the silver mirror. Since the recorded interferogram is not an ideal cosine response, higher order harmonics are present in the obtained spectrum. The appearance of the second harmonic defines the free spectral range of the spectrometer and limits the operating range.

The operating range is an important parameter. The upper limit of the operating range is defined by the visibility of the spectrometer, which depends on the spectrometer type and the optical properties of the i-layer material. For the standing wave spectrometer with an amorphous silicon transparent photodetector, the visibility is limited to 380-800 nm. On the other hand, for the Fabry-Perot spectrometer with an amorphous silicon transparent photodetector, the visibility is limited to 310-750 nm. The lower limit of the operating range is determined by the free spectral range and broadening of spectral lines due to the finite recording region (Eq. (3.40)). In practical applications, for a Fabry-Perot spectrometer with low reflectivity reflectors, it can be assumed that higher order harmonics are suppressed. In such a case, the lower operating limit is also determined by the spectrometer visibility.

The operating range of the standing wave and Fabry-Perot spectrometer can be shifted to other regions of the optical spectrum, by using materials with different energy band gaps. For a crystalline silicon transparent photodetector, the operating range can be shifted to the near infrared part of the optical spectrum (Fig. 2.2a). The upper limit in this case is almost 1100 nm, but due to the free spectral range and broadening of spectral lines, the lower operating limit is higher than 550 nm.

Another important property of the spectrometer device is the accuracy. To accurately determine the light spectrum using a Michelson spectrometer, the Fourier transform of the recorded interferogram has to be normalized by the spectrometer visibility and number of sampling points. For the standing wave and Fabry-Perot spectrometer, this is not the case. Since their recorded interferogram deviates from the cosine function, their accuracy is influenced by the Fourier series components. For the standing wave spectrometer, the interferogram deviations are wavelength dependent, since Fabry-Perot oscillations are influencing the absorption of the i-layer. For the Fabry-Perot spectrometer, the deviations are independent on the wavelength. Consequently, for the Fabry-Perot spectrometer, the error due to the Fourier components is the same for all wavelengths, and the accuracy of the determined spectrum is the same as for the Michelson spectrometer. On the other hand, the standing wave spectrometer exhibits reduced accuracy since the Fourier components are wavelength dependent.

The main advantage of the standing wave spectrometer over the Fabry-Perot spectrometer is the strength of the generated signal. Since only the AC photocurrent carries information about the spectrum, it is important that the AC photocurrent is as large as possible compared to the DC photocurrent. The DC photocurrent can be considered as a noise of the spectrometer device [59]. For the standing wave (Fig. 3.33a) and Fabry-Perot spectrometer (Fig. 3.29a), the DC photocurrents are comparable. Therefore, the measure of the signal strength is given by the selectivity
of the spectrometer, which represents the ratio between the AC and DC photocurrent. The selectivity of the standing wave spectrometer is larger than for the Fabry-Perot, due to the reflectivity of a mirror. To improve the selectivity of the Fabry-Perot spectrometer, reflectors with higher reflectivity can be used. At the same time, this will reduce the operating range of the Fabry-Perot spectrometer. The high reflectivity of the reflectors increase the deviations of the recorded interferogram, and the second order harmonic is more pronounced [54, 56]. Consequently, the free spectral range and the broadening of spectral lines have to be taken into account when determining the lower operating range of the Fabry-Perot spectrometer with high reflectivity of the reflectors.

The resolution of the standing wave and Fabry-Perot spectrometer is determined by the effective recording length according to Eq. (3.38). By taking into account the partially coherent light source, the resolution of the standing wave and Fabry-Perot spectrometer is two times smaller than for the Michelson spectrometer. This is influenced by the linear setup of the spectrometers. Due to the linear configuration of the spectrometers, the maximum effective recording region is half of the value that can be achieved with the Michelson spectrometer. The effective recording length is determined by the coherence length of the light and the minimum distance between the transparent detector and the mirror (reflectors). To properly record the interferogram, the minimum distance should be as small as technically possible and the recording length should be in range of 20 $\mu$m.
3. Transparent photodetector - applications
Part III

Optoelectronic devices with nano-structured interfaces
Chapter 4

Silicon thin-film solar cells

The technological advantages of silicon thin-film solar cells are numerous. Thin-film technologies are compatible with substrates that have an area larger than 1 m$^2$ [66, 67]. Furthermore, thin-films are deposited at low temperatures, which allows for the use of substrates such as glass or plastic [24, 25]. The thickness of silicon thin-film solar cells is usually smaller than 3 µm [68, 69], which results in significant reduction of material costs. However, the main disadvantage of the silicon thin-film solar cells is that their energy conversion efficiencies are low compared to c-Si wafer based solar cells.

To reduce the gap between the silicon thin-film and c-Si wafer based solar cells, efficient light trapping schemes are developed. Recently, substrates with periodic textures [33, 68, 69], multiscale textures [52, 70–72] and nanowire architecture [73, 74] have been implemented successfully resulting in improved conversion efficiencies of silicon thin-film solar cells. To further optimize the light trapping, the surface textures are analyzed by image processing algorithms [75], and optical simulations are used to calculate the wave propagation within the solar cells for different surface textures [76–79]. Furthermore, different approaches to determine how deposition of silicon thin-films influences the surface textures are also developed [80–83]. By combining these approaches, the performances of silicon thin-film solar cells can be improved, and their position on the market can become more competitive.

The aim of this chapter is to provide some fundamentals about solar cells with focus on the silicon thin-film solar cells. In the beginning of the chapter, characteristic parameters of the solar cells are introduced. Furthermore, different configurations of the silicon thin-film solar cells are presented together with common approaches to introduce the light trapping and to model the silicon film formation. In the end, the numerical method used to solve Maxwell’s equations and analyze the electromagnetic wave propagation in silicon thin-film solar cells is described and compared to the analytical methods from Sec. 2.3.2.

4.1 Solar cells - fundamental concepts

Solar cells are optoelectronic devices developed to generate electrical power when illuminated by sunlight. In general, solar cells are p-n or p-i-n photodiodes [38, 84]. Therefore, the fundamental considerations about photon detectors (Sec. 2.1) and photodiodes (Sec. 2.2.1) are also valid in this case. The solar radiation is absorbed in solar cells generating electron-hole pairs. The built-in electric field separates gener-
Figure 4.1: (a) Equivalent circuit, (b) current-voltage characteristic and (c) generated power for an ideal solar cell.

ated charge carriers and creates a photocurrent. Therefore, the equivalent circuit of an ideal solar cell under illumination (Fig. 4.1a) can be described by the parallel connection of a diode and current source that represents generated photocurrent [38, 84]. Consequently, the current of the ideal solar cell \( I_d \) is given by [38, 84]:

\[
I_d = I_{sat} \left( \exp \left( \frac{qV_d}{k_B T_{abs}} \right) - 1 \right) - I_{tot}^{ph}
\]  

(4.1)

where \( I_{sat} \) is the saturation current, \( I_{tot}^{ph} \) is the total generated photocurrent, \( V_d \) is the applied voltage, \( k_B \) is Boltzmann constant, and \( T_{abs} \) is the absolute temperature of the solar cell. The current-voltage characteristic and generated power of the ideal solar cell can be obtained from Eq. (4.1).

Figure 4.1 schematically depicts the equivalent circuit (Fig. 4.1a), current-voltage characteristic (Fig. 4.1b) and generated power (Fig. 4.1c) of the ideal solar cell. From Fig. 4.1b, important parameters such as short circuit current \( I_{sc} \) and open circuit voltage \( V_{oc} \) can be determined. The short circuit current represents the current of the solar cell when zero voltage is applied. The open circuit voltage is the voltage applied to the solar cell for which the generated current is zero. For an ideal solar cell, the short circuit current and open circuit voltage are given by [84]:

\[
I_{sc} = I_{tot}^{ph}
\]  

(4.2)

\[
V_{oc} = \frac{k_B T_{abs}}{q} \ln \left( \frac{I_{tot}^{ph}}{I_{sat}} + 1 \right)
\]  

(4.3)

The generated power curve (Fig. 4.1c) is obtained from the current-voltage characteristic (\( P = -I_d V_d \)). Figure 4.1c shows that the solar cell generates power for voltages larger than zero, but smaller than the open circuit voltage (\( 0 < V_d < V_{oc} \)). The power curve is used to determine the maximum generated power \( P_{max} \). To
produce maximum energy, the solar cell should be connected to the load given by:

\[ R_{ch} = -\frac{V_{mp}}{I_{mp}} \]  

(4.4)

where \( V_{mp} \) and \( I_{mp} \) are the maximum power voltage and current \((P_{max} = -I_{mp}V_{mp})\), and \( R_{ch} \) is the characteristic resistance of the solar cell. For the maximum power point, the conversion efficiency of the solar cell is also maximum. The maximum conversion efficiency of the solar cell for a known input power \((P_{in})\) is given by [84]:

\[ \eta_{ce}^{\max} = \frac{I_{mp}V_{mp}}{P_{in}} \]  

(4.5)

Another important parameter of the solar cell is the fill factor \((FF)\). The fill factor is the measure of how much the current-voltage characteristic of the solar cells resembles a rectangular shape [84]. For the rectangular characteristic, the solar cell would produce constant current equal to the short circuit current for all voltages smaller than the open circuit voltage. The fill factor \((FF)\) is defined as [84]:

\[ FF = \frac{I_{mp}V_{mp}}{I_{sc}V_{oc}} \]  

(4.6)

The maximum value that the fill factor can achieve is one. The fill factor is often used to express the conversion efficiency using the short circuit current and open circuit voltage [84]:

\[ \eta_{ce}^{\max} = \frac{I_{sc}V_{oc}FF}{P_{in}} \]  

(4.7)

The current-voltage characteristic and generated power of a solar cell is influenced by the input power of the solar radiation \((P_{in})\). The solar radiation that reaches the solar cell depends on its position defined by altitude, latitude and longitude. Furthermore, the solar radiation is not constant during the year. Therefore, to eliminate these variations in experimental measurements, standard spectral densities for sunlight have been introduced [85, 86]. Generally accepted standards are formulated by the American Society for Testing and Materials and published in the document ASTM G-173-03 [87]. The spectral density of the solar radiation that reaches the earth’s atmosphere is called air mass zero (AM 0) (Fig. 4.2), where the value zero quantifies the atmosphere thickness through which radiation is passing. To characterize the solar cells, it is more suitable to use the spectral density of the solar radiation that reaches the earth’s surface. For this case, the air mass is defined by the angle \((\theta)\) between the position of the sun and the zenith [84]:

\[ AM = \frac{1}{\cos \theta} \]  

(4.8)

Based on Eq. (4.8), thickness of one air mass corresponds to \(0^\circ\) angle, and thickness of 2 air masses corresponds to \(60^\circ\) angle. The standard spectral density that is used for characterization of solar cells is air mass 1.5 (AM 1.5) (Fig. 4.2). AM 1.5 spectral density corresponds to an angle of \(48.2^\circ\) with total intensity of \(1 \text{ kW/m}^2\) [88].

Figure 4.2 exhibits spectral densities for AM 0 and AM 1.5. To describe AM 0 curve, the black body radiation can be used. On the other hand, AM 1.5 spectral density is influenced by the earth’s atmosphere. For shorter wavelengths, AM 1.5 is lower compared to AM 0 due to the scattering of the light by the molecules and particles in the earth’s atmosphere. For longer wavelengths, AM 1.5 exhibits absorption bands, which are caused by the absorption of the gases that constitute the atmosphere.
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Figure 4.2: Spectral density of solar radiation for air mass zero and air mass 1.5.

Figure 4.3: Equivalent circuit of solar cell with parasitic resistances.

**Series and shunt resistance.** When analyzing performances of a real solar cell, parasitic resistances have to be taken into account. Every solar cell exhibits parasitic series and shunt resistance, which influence the fill factor and conversion efficiency of the solar cell. The shunt resistance \( R_{sh} \) arises from leakage currents within the solar cell junction and along the edges of the solar cell. The main contributors to the leakage current within the junction region are defects and impurities [84], while surface effects are responsible for leakage along the edges [38]. The series resistance \( R_s \) is influenced by the bulk resistance of the materials used to produce the solar cell and the electric contacts, and by the contact resistance between different materials [38, 84]. Figure 4.3 schematically depicts the equivalent circuit of a realistic solar cell with parasitic resistances.

The current of the solar cell, where the parasitic resistances are taken into account, is given by [38]:

\[
I_d = I_{sat} \left( \exp \left( \frac{q (V_d - R_s I_d)}{k_B T_{abs}} \right) - 1 \right) + \frac{V_d - R_s I_d}{R_{sh}} - I_{ph} \tag{4.9}
\]

Equation (4.9) is transcendent, and it has to be solved numerically. Therefore, the following simplifications are used to determine the influence of the series and shunt resistance. The influence of the series resistance is shown by assuming that the shunt resistance is infinite \( R_{sh} = \infty \). To analyze the influence of the shunt resistance, the series resistance is neglected \( R_s = 0 \).

Figure 4.4 exhibits the influence of the series resistance on solar cell performances. The equivalent circuit is shown in Fig. 4.4a. The current-voltage characteristic is
4.2 Thin-film solar cells

Wafer based crystalline silicon solar cells are realized as p-n photodiodes, where the p- and n-region within the same silicon wafer are achieved by doping [23, 38, 84].
Since low temperature silicon thin-film solar cells are typically deposited by PECVD process [24, 28, 30, 41, 52, 66, 67, 89–97], their doped regions exhibit high density of defects and a short life time of photogenerated charge carriers [98, 99]. Therefore, silicon thin-film solar cells are typically produced as p-i-n photodiodes [22, 43, 94, 100]. The intrinsic i-layer exhibits low defect density, and the life time of generated charge carriers is increased [22, 43, 100]. This allows for the separation of charges by the built-in electric field and their transport to the solar cell front or back contact, where they are collected.

### 4.2.1 Solar cell configurations

Fabrication of silicon thin-film solar cells can be achieved either in substrate or superstrate configuration (Fig. 4.6). For the substrate configuration solar cells (Fig. 4.6a), the fabrication starts from the back contact. The back contact is formed on top on a glass or plastic substrate. On top of the back contact, the n-i-p layer sequence of the solar cell is then deposited, followed by the front contact. Due to the layer sequence deposition, the substrate configuration solar cells are also called n-i-p solar cells. For the superstrate configuration solar cells (Fig. 4.6a), the fabrication starts from the front contact. In this case the front contact is deposited on a glass substrate, followed by p-i-n layer sequence and the back contact. The superstrate configuration solar cells are also called p-i-n solar cells.

Figure 4.6 schematically depicts different configurations of thin-film solar cells. The substrate configuration is shown in Fig. 4.6a. For this configuration the light directly enters the solar cell through the front contact. Figure 4.6b depicts the superstrate configuration, where the light has to pass through the glass substrate and the front contact to enter the solar cell. The front contact has to be conductive to collect the generated charge carriers and transparent to allow the light to enter the solar cell. In general, a TCO layer is used as a front contact of the solar cells.
irrespective of their configuration. TCO materials typically used for the front contact of solar cells are: ZnO:Al, boron doped zinc oxide (ZnO:B), SnO$_2$:F or ITO [45, 52, 70, 71, 90, 94, 101, 102]. The optical properties of ZnO:Al and SnO$_2$:F are already shown in Sec. 2.2.2 (Fig. 2.2b).

Part of the light that enters the solar cell gets absorbed, and part of it reaches the back contact. Consequently, the back contact has to be reflective so that the light is reflected back into the solar cell. Furthermore, the back contact has to be conductive to collect generated charge carriers. The back contact can be composed of a back reflector with or without a TCO buffer layer [103, 104]. Silver, aluminum or white paint are commonly used as back reflectors in silicon thin-film solar cells [31–33, 66–68, 89, 95–97, 101, 105–112]. Each of these materials has advantages and disadvantages. For example, silver exhibits excellent optical properties in the visible region of the optical spectrum [65], and its electrical properties allow for an increased collection of generated charge carriers. However, silver is expensive. As an alternative, aluminum can be used. The optical properties of aluminum are not as good as those of silver [65], but its electrical properties also allow for increased collection of generated charges. Due to their good electrical properties, silver and aluminum can be used as back reflectors without a TCO buffer layer. The white paint behaves optically as a quasi-Lambertian scatterer, which is good for light trapping [31, 33, 112, 113]. However, the white paint is not conductive, and a back TCO layer with thickness larger than 2 $\mu$m has to be employed in order to collect the charges [31, 33]. For the metal back reflector, ZnO:Al is typically used as the buffer layer material [66, 69, 89, 93, 95–97, 101, 105, 109, 114–118]. For the white paint reflectors, ZnO:B deposited by low pressure chemical vapor deposition (LPCVD) process is used to form the buffer layer [31–33]. Recently, different dielectrics such as silicon-oxide [111, 119, 120] or magnesium fluoride (MgF$_2$) [121, 122] have been investigated for this purpose.

Silicon thin-film solar cells are based on a-Si:H and $\mu$c-Si:H materials, which exhibit good optical properties in the visible region of the electromagnetic spectrum (Fig. 2.2a). Silicon thin-film solar cells can be fabricated either as single junction or
Figure 4.7: Silicon thin film solar cells. (a) Amorphous and (b) microcrystalline silicon single junction solar cell. (c) Micromorph tandem silicon solar cell.

As micromorph tandem solar cells (Fig. 4.7). Single junction solar cells are based on a single a-Si:H or µc-Si:H p-i-n photodiode (Figs. 4.7a and 4.7b), while the micromorph tandem solar cells are based on a stacked a-Si:H and µc-Si:H p-i-n photodiodes (Fig. 4.7c).

Figure 4.7 schematically depicts a-Si:H and µc-Si:H single and tandem solar cells in superstrate configuration where the back contact is composed of a metal reflector and TCO buffer layer. The typical thickness of the buffer layer in combination with a metal reflector is around 100 nm [66, 69, 89, 93, 95–97, 101, 105, 109, 114–118]. On the other hand, the thickness of the front TCO layer should be large enough to achieve sufficient lateral conductivity for transport of the charge carriers, and it can range from 0.5 µm to 5 µm [45, 102, 105]. The doped p- and n- region of thin-film silicon solar cells should be thin. Due to the high defect density in the doped regions, the charge carriers generated in the p- and n- layer do not contribute to the generated photocurrent (Sec. 2.2.1). Consequently, it can be assumed that the light absorbed in these layers contributes only to losses. The thickness of the p- and n-layer is typically in the range of 10-30 nm [123].

The thickness of the i-layer depends on the silicon material. A single junction a-Si:H solar cell is shown in Fig. 4.7a. Due to Staebler-Wronski effect [124], the thickness of the i-layer of a-Si:H solar cells is typically around 300 nm [29, 31, 33, 66, 67, 89, 114]. Staebler-Wronski effect states that the a-Si material exhibits additional defects under illumination. These defects act as recombination centers for the photogenerated charge carriers. Consequently, the conversion efficiency of the solar cell is reduced. By limiting the i-layer thickness of a-Si solar cell, the influence of Staebler-Wronski effect is reduced. Due to the small thickness of the i-layer, the short circuit current density of a-Si solar cell is in the range of 15-17 mA/cm² [33, 66].

Figure 4.7b depicts a µc-Si solar cell with typical thicknesses of individual layers. Unlike a-Si solar cells, the i-layer thickness of µc-Si solar cells is in the range of 1-3 µm, and the short circuit current density is larger than 24 mA/cm² [68, 69, 97, 118].
Although $\mu c$-Si solar cells exhibit larger short circuit current densities, the conversion efficiencies of $\mu c$-Si and a-Si solar cells are comparable since a-Si solar cells have larger open circuit voltages [28–30, 33, 68, 69].

To improve the properties of silicon thin-film solar cells, a concept of stacking single junction solar cells have been implemented. Figure 4.7c depicts micromorph tandem solar cell. In micromorph tandem solar cells, an a-Si solar cell is placed next to the front contact and a $\mu c$-Si solar cell next to the back contact. The top a-Si solar cell is used to generate photocurrent for shorter wavelength light, while the bottom $\mu c$-Si solar cell is used to generate photocurrent for longer wavelength light. Due to the stacking of photodiodes, a tandem solar cell exhibits increased open circuit voltage [29]. In order to maximize the conversion efficiency of micromorph tandem solar cells, it is necessary to match the currents of the top and bottom solar cell [41]. If the currents are not matched, the overall current is limited by the solar cell that generates lower photocurrent. One of the approaches to improve the overall photocurrent is by introducing interlayer reflector (Fig. 4.7c) between the stacked solar cells [125, 126]. As interlayer reflectors, TCOs such as ZnO and hydrogenated silicon oxide (SiO$_x$:H) have been proposed [126–129].

To achieve high short circuit currents and conversion efficiencies of silicon thin-film solar cells, light trapping (photon management) is required. The goal of light trapping is to confine the light within the absorption layer of the solar cell. The most common way to introduce light trapping is by texturing the surface of the solar cell contacts as shown in Figs. 4.6 and 4.7. Due to the textured surface, the light gets scattered/diffracted, and the optical path length within the absorber layer is increased. As a consequence, the absorption within the solar cell is improved, which results in a higher short circuit current and conversion efficiency.

The influence of light trapping on the short circuit current can be determined by comparing silicon solar cells deposited on textured and smooth substrates. Experimental investigation showed that a-Si solar cells prepared on textured substrates exhibit increase of short circuit current density by 27 % compared to solar cells prepared on smooth substrates [93]. For $\mu c$-Si solar cells, the effect is even more pronounced, and the short circuit current density increases by almost 50 % due to the surface texturing [50].

Light trapping in substrate configuration solar cells is achieved by texturing the back contact. The textured back contact can be realized by deposition of a metal back reflector on a textured substrate [68, 118], which is schematically depicted in Fig. 4.6a. An alternative approach is by direct deposition of a textured metal back reflector [97]. To introduce light trapping in superstrate configuration solar cells, textured front contact is used (Fig. 4.6b). For this purpose, different types of randomly textured TCOs have been developed [45, 52, 70, 71, 90, 101, 102].

### 4.2.2 Randomly textured transparent conductive oxides

Randomly textured TCO front contacts can be fabricated using different approaches. Textured ZnO:B and SnO$_2$:F are realized by direct deposition using LPCVD and APCVD process, respectively [28, 45, 51, 52, 70, 71, 102, 130]. On the other hand, textured ZnO:Al substrates are realized by wet etching of sputtered films [50, 75, 89, 90, 131]. The surface features of randomly textured substrates depend on the fabrication process. The surface of LPCVD ZnO:B and APCVD SnO$_2$:F exhibits
pyramid-like features [28, 45, 51, 52, 70, 71, 102, 130], while etched ZnO:Al substrates exhibit crater-like features [50, 75, 89, 90, 131]. To characterize randomly textured substrates, various experimental and theoretical methods have been proposed. Experimental measurements are used to determine the haze and angular distribution function (ADF) of textured substrates [52, 132, 133]. The haze parameter is defined as the ratio of the diffused and total transmission through a textured substrate, and represents the total amount of light that is scattered/diffracted. On the other hand, ADF determines the amount of light that is scattered/diffracted by a textured substrate at a certain angle. The haze and ADF parameters are typically measured in air, and they cannot be directly correlated to solar cell properties. To overcome this problem, the scattering properties of textured substrates coated with silicon materials are in the focus of recent investigation [134]. The scattering properties can also be determined from an atomic force microscopy (AFM) measurement of a textured substrate by treating its surface as a phase mask and applying Fourier transform [133, 135]. To obtain the solar cell properties such as quantum efficiency and short circuit current, the haze and ADF parameters can be implemented in scattering models and combined with optical simulations [136]. Alternatively, AFM measurements of randomly textured substrates can be analyzed by image segmentation algorithms to determine the dimensions of individual surface features [75]. To determine the solar cell parameters, the surface textures are then approximated by geometrical shapes and implemented in optical simulations.

In this study, an image segmentation algorithm is used to analyze and characterize randomly textured SnO$_2$:F and wet etched ZnO:Al. Furthermore, the surface textures of these substrates are approximated with different geometrical shapes in order to create an adequate optical model of the front contact.

**Randomly textured SnO$_2$:F substrate.** Randomly textured SnO$_2$:F substrates are commercially produced by companies such as Asahi Glass and Nippon Sheet Glass. Textured SnO$_2$:F substrates are typically used for fabrication of a-Si:H single and micromorph tandem solar cells [29, 66, 93, 114, 137]. Figure 4.8 depicts the surface of randomly textured SnO$_2$:F substrate obtained by AFM measurement. The fabrication and measurement of the substrate have been realized at Nippon Sheet Glass company. Although the complete area of the AFM measurement is 10 x 10 µm$^2$, Fig. 4.8 depicts only 2.5 x 2.5 µm$^2$ so that the surface textures are better visualized. The surface textures of SnO$_2$:F substrate exhibit pyramid like shape with different lateral dimensions and heights.

To determine individual features of randomly textured SnO$_2$:F, an image segmentation algorithm is applied to AFM measured surface. For pyramid like features, the algorithm first detects all local maximum points (pyramid tips) and then determines boundaries between individual features. After segmentation is complete, the areas and average heights of individual features are obtained. To determine the lateral dimensions of the features, it is assumed that the features can be approximated by square base pyramids, which ensures complete surface coverage.

Figure 4.9 depicts extracted dimensions of individual features in the case of the textured SnO$_2$:F substrate. The lateral size of the features varies from 100 nm to 600 nm, while their height is in the range of 20-200 nm. The average ratio between the height and period of the individual features is 0.27, which is depicted by a red line in Fig. 4.9. To investigate the accuracy of the assumption that the features
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Figure 4.8: Randomly textured SnO$_2$:F substrate [138]. Top view (left) and side view (right).

Figure 4.9: Extracted dimensions of individual features of randomly textured SnO$_2$:F substrate (blue circles) and average height to period ratio (red line).

can be approximated by square base pyramids, an artificial quasi-random substrate is created. The individual features of randomly textured substrate are replaced by square base pyramids with constant height to period ratio of 0.27.

Figure 4.10 depicts 2.5 x 2.5 $\mu$m$^2$ area of measured (Fig. 4.10a) and quasi-random SnO$_2$:F substrate (Fig. 4.10b). The root mean square (rms) roughness of the measured and quasi-random substrate is 38.4 nm and 40.3 nm, respectively, which is a good agreement. In order to make a detailed comparison, the power spectral density (PSD) of the measured and quasi-random substrate is calculated [82]. The PSD of a textured surface represents the surface roughness for a specific length scale or spatial frequency [139, 140]. To determine the PSD, first 2D Fourier transform has to be applied to the surface profile. The 2D PSD is then calculated as a square amplitude of the 2D Fourier transform divided by the surface area [141]. Finally, the PSD of a textured surface is obtained by azimuthal averaging of the 2D PSD [141].

Figure 4.11 depicts the PSD of the measured and quasi-random SnO$_2$:F substrate. Although the total rms roughness of these substrates is almost the same, the PSD shows that surface roughness is not equal for different spatial frequencies. However, the agreement between the measured and quasi-random surface is relatively good. It can be concluded that representing individual features of randomly textured SnO$_2$:F
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![Figure 4.10](image)

Figure 4.10: (a) Textured SnO$_2$:F substrate [138] and (b) pyramidal approximation.

![Figure 4.11](image)

Figure 4.11: Power spectral density of measured and artificial SnO$_2$:F substrate.

substrate by square base pyramids with a height to period ratio of 0.27 is a good modeling approach. From the quasi-random substrate, the average values of the period and height can be determined. The average period is determined from the periods of all individual features by using an area-weighted function, and it is calculated to be 400 nm. From the average height to period ratio, the average height of 108 nm is calculated.

**Wet etched ZnO:Al substrate.** Randomly textured ZnO:Al substrates are mostly used for fabrication of $\mu$c-Si:H single and micromorph tandem solar cells [30, 89, 105, 137, 142]. Textured ZnO:Al substrates are realized in a two step process. First, ZnO:Al film is deposited by an RF magnetron sputtering, and then it is wet etched in diluted hydrochloric (HCl) or hydrofluoric (HF) acid [50, 75, 131]. The textures of etched ZnO:Al films exhibit crater like shape, where the dimensions of the craters depend on the acid used for etching and the etching time itself [50, 75, 89, 90, 131].

Figure 4.12 depicts the surface of ZnO:Al film etched with HCl acid for 40 s, which is measured by AFM. The fabrication and measurement of the substrate have been realized at Jülich Research Center [144]. The complete area of the AFM measurement is 15 x 15 $\mu$m$^2$, but Fig. 4.12 depicts 5 x 5 $\mu$m$^2$ for better visualization of the surface.
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textures. The size of the surface textures of the ZnO:Al substrate is much larger compared to the SnO\textsubscript{2}:F substrate (Fig. 4.8). Again, to determine the size of the individual features, an image segmentation algorithm is used.

The depth and diameter of the individual craters of etched ZnO:Al substrate are depicted in Fig. 4.13. For crater like features, the image segmentation algorithm first detects all local minimum points (crater bottoms) and then determines borders between craters. To determine the dimension of surface textures, it is assumed that the craters can be approximated by inverted cones in hexagonal arrangement to ensure complete surface coverage. The diameters of the craters vary from 250 nm to 2 \(\mu\)m, while their depths vary from 50 nm to more than 400 nm. The average ratio between the depth and diameter of the craters is 0.18, which is shown by the red line in Fig. 4.13.

Figure 4.14 shows measured etched ZnO:Al substrate and corresponding quasi-random substrate. For the quasi-random substrate, the individual craters are replaced by inverted cones with constant depth to diameter ratio of 0.18. The rms roughness of the quasi-random and measured etched ZnO:Al substrate is almost equal. The rms roughness of the measured substrate (Fig. 4.14a) is 116 nm, while the rms roughness of the quasi-random substrate (Fig. 4.14b) is 113 nm.
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Figure 4.14: (a) Etched ZnO:Al substrate [143] and (b) cone approximation.

Figure 4.15: Power spectral density of measured and artificial etched ZnO:Al substrate.

Figure 4.15 depicts comparison of the PSD for the measured and quasi-random etched ZnO:Al substrate. The agreement between the substrates is very good for small spatial frequencies (large dimensions). For the larger spatial frequencies (smaller dimensions), the surface roughness of the quasi-random substrate is reduced compared to the measured substrate. Nevertheless, representing individual features of etched ZnO:Al substrate by inverted cones is a good approximation. Furthermore, the average crater diameter is determined to be 1732 nm, where an area-weighted averaging is used. From the average depth to diameter ratio, the average crater depth is calculated to be 315 nm.

4.2.3 Formation of silicon films on textured substrates

When depositing silicon thin-film solar cells on randomly textured substrates, the surface textures of the substrates propagate through the solar cell layers. Consequently, the surface of the deposited solar cells is also textured. Determining the surface textures of the deposited solar cells is necessary for better understanding and optimization of light trapping. Due to their small thickness, most common approach in literature assumes that the surface textures of deposited silicon thin-film solar cells are the same.
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Figure 4.16: Surface textures of (a) textured SnO$_2$:F substrate and (b) deposited a-Si:H solar cell [143].

as that of the textured substrates [66, 92, 145–147]. However, experimental measurements show that the surface textures are different [68, 69, 74, 95, 118, 148, 149].

Figure 4.16 depicts the surface textures of a randomly textured SnO$_2$:F substrate and an a-Si:H solar cell deposited on top. The fabrication of the a-Si:H solar cell and the AFM measurements have been realized at Jülich Research Center [144]. The thickness of the a-Si:H is 300 nm, which is typical thickness for this type of silicon thin-film solar cells (Fig. 4.7a). The a-Si:H solar cell is deposited by a PECVD process using a gas mixture of silane and hydrogen. The deposition is realized at a deposition pressure of 133 Pa and at a substrate temperature of 260 °C [82, 144]. The surface morphologies of the substrate (Fig. 4.16a) and the deposited a-Si:H solar cell (Fig. 4.16b) have been measured by the AFM for exactly the same area. The alignment for these measurements is achieved using special laser markers [81, 82, 144]. The measured surface of the deposited a-Si:H solar cell reveals that the lateral dimensions of surface textures are smoother and larger compared to that of the substrate. The smoothing occurs for the peak points of the substrate, which are located at the tips of the pyramid like features. Since the surface textures of SnO$_2$:F substrate are relatively small (Fig. 4.9), the surface textures with higher peak points merge with surrounding features leading to larger surface textures. The observed changes of the surface textures are influenced by the uniform formation of the a-Si:H silicon film.

The influence of silicon film formation on changes of the surface textures depends on the type of the textured substrate and silicon material. The surface textures of an etched ZnO:Al substrate and a deposited $\mu$c-Si:H solar cell for the same area are shown in Fig. 4.17. The fabrication of the etched ZnO:Al substrate, the deposition of $\mu$c-Si:H solar cell and the AFM measurements have been realized at Jülich Research Center [144]. The thickness of the deposited solar cell is 1000 nm, which is in the typical thickness range of single junction $\mu$c-Si:H solar cells (Fig. 4.7b). The deposition process is the same as for a-Si:H solar cell, but with different deposition conditions. The $\mu$c-Si:H solar cell is deposited at a pressure of 1333 Pa and at a substrate temperature of 260 °C [82, 144]. Again, the surface of the etched ZnO:Al substrate (Fig. 4.17a) and deposited $\mu$c-Si:H solar cell (Fig. 4.17b) have been measured by the AFM using laser markers [144]. The surface textures of the $\mu$c-Si:H solar cell are smoother for the peak points of the substrate, which are now located at the crater edges. Since the dimension of the craters are large (Fig. 4.13), there is no significant change in their
Figure 4.17: Surface textures of (a) etched ZnO:Al substrate and (b) deposited $\mu$-c-Si:H solar cell [143].

size after the deposition of the solar cell. The surface textures of the deposited solar cell also exhibit nanotextures, which appear due to the columnar structure of $\mu$-c-Si:H film [43, 150]. Consequently, the formation of $\mu$-c-Si:H films is more directional than that of a-Si:H films [150].

In recent years, several different methods to determine the realistic surface textures of the deposited silicon thin-film solar cells have been developed [80–83]. The common assumption in these methods is that the formation of the silicon films deposited by PECVD process can be described by the direction of the local surface normal. As a part of this study, a surface coverage algorithm is developed in order to calculate the realistic surface morphologies of deposited a-Si:H and $\mu$-c-Si:H solar cells [81, 82]. The different film morphologies that the algorithm can model are shown in Fig. 4.18.

Figure 4.18a depicts the surface coverage algorithm used to determine the surface textures of deposited silicon thin-film solar cells. The input parameters of the surface coverage algorithm are the substrate morphology and nominal film thickness (d). To obtain the morphology of the deposited film, the surface coverage algorithm first determines the local surface normal for each substrate point. In the next step, the film thickness ($d(\alpha, K)$) is calculated for each substrate point assuming that it depends on the angle between the local surface normal and glass substrate normal ($\alpha$) as shown in Fig. 4.18a. This dependance is described by the direction factor (K). The film thickness is equal to the nominal value (d), if the local surface normal is parallel to the substrate normal ($\alpha = 0^\circ$). On the other hand, if the local surface normal is orthogonal to the glass substrate normal ($\alpha = 90^\circ$), the film thickness is reduced to $d \cdot K$. After the film thickness is determined, it is applied in a direction given by the local surface normal for the corresponding substrate point, and the surface point of the deposited film is obtained. Depending on the substrate morphology, for some $x$- and $y$-coordinates several surface points of the deposited film can be calculated. For such cases, the surface coverage algorithm selects the highest calculated film point. As a consequence, the surface coverage algorithm cannot predict the formation of holes or voids in the deposited film.

The uniform film deposition is shown in Fig. 4.18b. For this case, the direction factor is equal to one, and the film thickness is independent of the angle between the local surface normal and glass substrate normal. Consequently, the film thickness in the direction of the local surface normal is equal to the nominal value (d) for
Figure 4.18: (a) Surface coverage algorithm. Different film morphologies obtainable by the surface coverage algorithm: (b) uniform, (c) without changes and (d) flat.

every substrate point. For the uniform film formation, the surface textures become smoother, which occurs for the substrate peak points. Furthermore, the film thickness in the direction of the glass substrate normal depends on the surface textures. For the substrate peak points, the film thickness is equal to the nominal value. On the other hand, for the substrate valley points, the film thickness is larger than the nominal value. Consequently, the uniform film formation allows for the surface textures to merge.

Figures 4.18c and 4.18d schematically depict film morphologies for extreme values of the direction factor. For a direction factor equal to zero (Fig. 4.18c), the film is only formed in the direction of the glass substrate normal. Consequently, there is no coverage of the side walls, and surface textures propagate unchanged through the deposited film. On the other hand, for very large value of the direction factor, a flat film morphology is obtained (Fig. 4.18d). For this case, all surface textures are merged together, and the film thickness is equal to the nominal value only for the highest substrate point.

Modeling the surface textures of silicon thin-film solar cells. To model the surface textures of a-Si:H solar cells deposited on a randomly textured substrate, the uniform approach can be used. Therefore, the direction parameter should be one. The input parameters for the surface coverage algorithm are the measured surface of the textured SnO₂:F substrate (Fig. 4.16a) and a nominal film thickness of 300 nm. A comparison of the measured and calculated surface is shown in Fig. 4.19. The measured morphology of a-Si:H solar cell is shown in Fig. 4.19a, while the simulated
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Figure 4.19: (a) Measured [143] and (b) simulated surface of a-Si:H solar cell deposited on a textured SnO$_2$:F substrate

Figure 4.20: Power spectral density of measured and simulated morphology of a-Si:H solar cell deposited on textured SnO$_2$:F substrate.

morphology is shown in Fig. 4.19b. The measured and the simulated surface exhibit a very good agreement. The rms roughness of the measured surface is 34.5 nm, while the simulated surface exhibits roughness of 33.8 nm. A detailed comparison is obtained using PSD approach.

Figure 4.20 depicts the PSDs of the measured and simulated a-Si:H solar cell surface. A good agreement between measurement and simulation is observed for all spatial frequencies. The presented results confirm that the surface coverage algorithm accurately predicts the surface of deposited a-Si:H solar cells. However, the uniform approximation for a deposition of a-Si:H solar cells is only valid for small deposition rates. For high deposition rates, the direction factor has to be included in the model [80].

To determine the surface morphology of µc-Si:H solar cells it is necessary to take into account directional film formation and appearance of nanofeatures. However, the surface coverage algorithm is not able to model the formation of natural textures of µc-Si:H films. Therefore, the algorithm can only be used to model the surface textures that originate from the textured substrate. For this purpose, the directional factor is
Figure 4.21: Measured surface of $\mu c$-Si:H solar cell deposited on etched ZnO:Al substrate (a) with [143] and (b) without natural textures. (c) Simulated surface.

set to 0.75. The input substrate morphology is etched ZnO:Al substrate (Fig. 4.17a), and the input film thickness is 1000 nm.

Figure 4.21 exhibits comparison between the measured and simulated surface of a deposited $\mu c$-Si:H solar cell on an etched ZnO:Al substrate. The surface morphology of the $\mu c$-Si:H solar cell (Fig. 4.21a) can be described as a superposition of the substrate textures that propagate through the $\mu c$-Si:H film and nanofeatures that are formed during film growth. To allow for a direct comparison of the measured and simulated surface textures, the natural textures of the $\mu c$-Si:H are filtered out [151]. Figure 4.21b depicts the measured morphology of $\mu c$-Si:H solar cell without natural textures. The simulated morphology is shown in Fig. 4.21c. The simulated morphology exhibits a good agreement with the measured morphology without natural textures. The rms roughness of the measured surface with and without nanofeatures is 114 nm and 110 nm, respectively. The roughness of the simulated surface is 101 nm.

Figure 4.22 exhibits PSD comparison of the measured and simulated surface of the $\mu c$-Si:H solar cell deposited on etched ZnO:Al substrate. The surface coverage algorithm is able to predict the evolution of the substrate textures, which is confirmed by the agreement of the PSD for the simulated and measured surface without nanofeatures. Nevertheless, the accurate description of the surface of $\mu c$-Si:H solar cells requires that the formation of natural textures is taken into account. This is
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Figure 4.22: Power spectral density of measured (with and without nanofeatures) and simulated morphology of a \( \mu c \)-Si:H solar cell deposited on etched ZnO:Al substrate.

achieved in the model developed by Hertel et al. [83]. More details about silicon film formation and its influence on light trapping in silicon thin-film solar cells can be found in literature [79, 81, 82, 152, 153].

4.3 Numerical modeling of electromagnetic wave propagation

The most accurate approaches to determine light propagation are based on analytical methods (Sec. 2.3.2). However, these methods can only be used for optical devices with simple flat interfaces, and linear and isotropic materials. For optical devices with textured interfaces, numerical methods are used to solve Maxwell’s equations and determine light propagation. Furthermore, numerical methods should be used in cases when the relationships that characterize the material (Eqs. (2.18) and (2.19)) are not linear, or materials are not isotropic.

Several computational methods have been developed to solve Maxwell’s equations numerically [154–160]. These methods are using integral or differential form of Maxwell’s equations, which are then solved in time or frequency domain. Numerical methods that solve Maxwell’s equations in integral form are method of moments (MoM) and finite integration technique (FIT) [154, 155]. Most common methods that are applied to Maxwell’s equations in differential form are finite element method (FEM), transfer line method (TLM) and finite-difference time-domain (FDTD) [156–160]. Frequency domain methods are MoM and FEM [154, 158], while FIT, TLM and FDTD belong to time domain techniques [155–157, 159, 160].

In this study, a 3D FDTD Maxwell’s equations solver is used to determine the light propagation in silicon thin-film solar cells. The advantages of FDTD method are numerous [160]. FDTD method does not use calculations with matrices, which can limit the size of a simulated device model. FDTD is a time domain technique, and it is able to determine the impulse response of the simulated device. Therefore, only a single simulation is needed to determine a steady-state response of the simulated device over a wide band of frequencies. Furthermore, the sources of error in FDTD
method are well known and usually connected with space-time discretization. One of
the major sources of error are oblique interfaces within the simulated device, since
they cannot be aligned with Cartesian grid. For such cases, the accuracy of simulation
can be improved by using finer spatial mesh settings. Finally, the material properties
of the simulated device can be predefined and stored in a computer memory, which
reduces the simulation time.

In this section, basics of FDTD method are presented. Furthermore, FDTD
method is compared with the analytical methods (Sec. 2.3.2) on the example of silicon
thin-film solar cells with flat interfaces.

4.3.1 Finite-difference time-domain algorithm

The algorithm for FDTD method has been developed by K.S. Yee in 1966 [159]. The
algorithm starts from Faraday’s and Ampere’s law given by Eqs. (2.22) and (2.23),
respectively (Sec. 2.3.1). To describe FDTD algorithm, Eqs. (2.22) and (2.23) should
be rewritten:

\[ \mu_0 \frac{\partial \mathbf{H}}{\partial t} = -\nabla \times \mathbf{E} \quad (4.10) \]
\[ \varepsilon_0 \varepsilon_r \frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{H} - \sigma \mathbf{E} \quad (4.11) \]

Equations (4.10) and (4.11) show the relationship between the electric and magnetic
component of an electromagnetic wave in their vector form. Assuming Cartesian
coordinate system, these vector equations can be expanded into a set of six scalar
equations - three for the electric and three for the magnetic component:

\[ \mu_0 \frac{\partial H_x}{\partial t} = \frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} \quad (4.12) \]
\[ \mu_0 \frac{\partial H_y}{\partial t} = \frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} \quad (4.13) \]
\[ \mu_0 \frac{\partial H_z}{\partial t} = \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} \quad (4.14) \]
\[ \varepsilon_0 \varepsilon_r \frac{\partial E_x}{\partial t} = \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} - \sigma E_x \quad (4.15) \]
\[ \varepsilon_0 \varepsilon_r \frac{\partial E_y}{\partial t} = \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} - \sigma E_y \quad (4.16) \]
\[ \varepsilon_0 \varepsilon_r \frac{\partial E_z}{\partial t} = \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - \sigma E_z \quad (4.17) \]

The numerical solution of the set of six equations (Eqs. (4.12)-(4.17)) requires
discretization in both space and time domain. Therefore, special notation have been
introduced to represent spatial and time coordinates [159, 160]. Space coordinates
are replaced by:

\[ (x, y, z) = (i \cdot \Delta x, j \cdot \Delta y, k \cdot \Delta z) \rightarrow (i, j, k) \quad (4.18) \]

where \( \Delta x, \Delta y \) and \( \Delta z \) are spatial steps in \( x, y \) and \( z \)-direction. In this notation, the
time is represented by:

\[ t = n \cdot \Delta t \rightarrow n \quad (4.19) \]
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\[ i = 0, \quad \frac{1}{2}, \quad 1, \quad \frac{3}{2}, \quad 2, \quad \frac{5}{2}, \quad 3, \quad \frac{7}{2}, \quad n = 0, \quad \frac{1}{2}, \quad 1, \quad \frac{3}{2}, \quad 2, \quad \frac{5}{2}, \quad 3, \quad \frac{7}{2} \]

Figure 4.23: Leap-frog algorithm. Space and time discretization for the electric and magnetic component of an electromagnetic wave.

where \( \Delta t \) is a time step. Furthermore, an arbitrary function of space and time is given by:

\[ u(x, y, z, t) = u(i \cdot \Delta x, j \cdot \Delta y, k \cdot \Delta z, n \cdot \Delta t) \rightarrow u^n_{i,j,k} \quad (4.20) \]

The basis of FDTD computation is a leap-frog algorithm, which is shown in Fig. 4.23. The leap-frog algorithm interleaves the electric and magnetic components of an electromagnetic wave at alternate spatial and time coordinates. In this configuration, the electric components are located at integer spatial and time coordinates, while the magnetic components are located at half-integer spatial and time coordinates. Furthermore, the leap-frog algorithm also defines the order of calculations. To determine the electric components at integer time step, the magnetic field components from previous half-integer time step are used. On the other hand, to calculate the magnetic field components at half-integer time step, the electric field components from the previous integer time step are used. The initial conditions of the leap-frog algorithm require that the electric and magnetic components are zero \( (E|^0 = 0 \text{ and } H|^{-1/2} = 0) \). The alternate computation of the electric and magnetic components ends when the convergence conditions are satisfied.

The discretization of the set of six equations (Eqs. (4.12)-(4.17)) starts by representing partial derivatives as finite differences \([159, 160]\). Due to the alternate spacing of the electric and magnetic components, the finite differences in space and time are different for the electric and magnetic components. The spatial derivatives are represented by:

\[ \frac{\partial u^n_{i,j,k}}{\partial x} = \begin{cases} \frac{u^n_{i+1/2,j,k} - u^n_{i-1/2,j,k}}{\Delta x} & \text{for magnetic components} \\ \frac{u^n_{i+1,j,k} - u^n_{i,j,k}}{\Delta x} & \text{for electric components} \end{cases} \quad (4.21) \]

while the time derivatives are given by:

\[ \frac{\partial u^n_{i,j,k}}{\partial t} = \begin{cases} \frac{u^{n+1/2}_{i,j,k} - u^{n-1/2}_{i,j,k}}{\Delta t} & \text{for magnetic components} \\ \frac{u^{n+1}_{i,j,k} - u^n_{i,j,k}}{\Delta t} & \text{for electric components} \end{cases} \quad (4.22) \]

The next step in the discretization of the set of six equations is to implement a 3D arrangement of the electric and magnetic components \([159, 160]\). This is done according
4.3 Numerical modeling of electromagnetic wave propagation

Figure 4.24: Cubic unit cell of Yee space lattice and the corresponding electric and magnetic components of an electromagnetic wave.

to Yee scheme (Fig. 4.24). Figure 4.24 schematically depicts the 3D spatial arrangement of the electric and magnetic components within the unit cell of space lattice as introduced by K.S. Yee [159, 160]. Again, the electric and magnetic components are calculated for an integer and half-integer time steps, respectively.

The finite difference approximation of the magnetic component in $x$-direction can be obtained by expanding Eq. (4.12) according to notation given by Eqs. (4.21) and (4.22):

$$
egin{align*}
\frac{H_{x_1}^{n+1/2} - H_{x_1}^{n-1/2}}{\Delta t} & = \frac{E_{y_1}^{n} - E_{y_1}^{n-1}}{\Delta z} - \frac{E_{z_1}^{n} - E_{z_1}^{n-1}}{\Delta y} \\
& = \frac{\Delta t}{\mu_0} \left( E_{y_1}^{n} - E_{y_1}^{n-1} \right) - \frac{\Delta t}{\mu_0} \left( E_{z_1}^{n} - E_{z_1}^{n-1} \right)
\end{align*}
$$

(4.23)

From Eq. (4.23), the magnetic component in $x$-direction at the next half-integer time step is given by:

$$
H_{x_1}^{n+1/2} = \frac{\Delta t}{\mu_0} \left( E_{y_1}^{n} - E_{y_1}^{n-1} \right) - \frac{\Delta t}{\mu_0} \left( E_{z_1}^{n} - E_{z_1}^{n-1} \right) + H_{x_1}^{n-1/2}
$$

(4.24)

For the magnetic components in $y$- and $z$-direction, the same procedure is applied to obtain the finite difference equations:

$$
egin{align*}
H_{y_1}^{n+1/2} & = \frac{\Delta t}{\mu_0} \left( E_{z_1}^{n} - E_{z_1}^{n-1} \right) - \frac{\Delta t}{\mu_0} \left( E_{x_1}^{n} - E_{x_1}^{n-1} \right) \\
& = \frac{\Delta t}{\mu_0} \left( E_{z_1}^{n} - E_{z_1}^{n-1} \right) - \frac{\Delta t}{\mu_0} \left( E_{x_1}^{n} - E_{x_1}^{n-1} \right)
\end{align*}
$$

(4.25)

$$
egin{align*}
H_{z_1}^{n+1/2} & = \frac{\Delta t}{\mu_0} \left( E_{x_1}^{n} - E_{x_1}^{n-1} \right) - \frac{\Delta t}{\mu_0} \left( E_{y_1}^{n} - E_{y_1}^{n-1} \right) \\
& = \frac{\Delta t}{\mu_0} \left( E_{x_1}^{n} - E_{x_1}^{n-1} \right) - \frac{\Delta t}{\mu_0} \left( E_{y_1}^{n} - E_{y_1}^{n-1} \right)
\end{align*}
$$

(4.26)
To determine the finite difference approximation for the electric component in \(x\)-direction, it is necessary to expand Eq. (4.15). By using the finite difference approximations of partial derivatives (Eqs. (4.21) and (4.22)), Eq. (4.15) can be approximated by:

\[
\epsilon_0 \sigma_{y|z+1/2,j,k}^n \frac{E_{x|z+1/2,j,k}^{n+1} - E_{x|z+1/2,j,k}^n}{\Delta t} = H_{y|z+1/2,j,k+1/2}^{n+1/2} - H_{y|z+1/2,j,k-1/2}^{n+1/2} - \Delta y \frac{H_{y|z+1/2,j,k}^{n+1/2} - H_{y|z+1/2,j,k-1/2}^{n+1/2}}{\Delta z} - \sigma_{z|z+1/2,j,k}^{n+1/2} \frac{E_{x|z+1/2,j,k}^{n+1} + E_{x|z+1/2,j,k}^n}{2} \quad (4.27)
\]

To express the electric component at the next integer time step from Eq. (4.27), it is necessary to estimate the value of the electric component at a half-integer time step. For that purpose, a semi-implicit approximation can be used [159, 160]:

\[
u_{z|z+1/2,j,k}^n = \frac{u_{z|z+1/2,j,k}^{n+1} + u_{z|z+1/2,j,k}^n}{2} \quad (4.28)
\]

Equation (4.27) can now be rewritten into:

\[
\epsilon_0 \sigma_{y|z+1/2,j,k}^n \frac{E_{x|z+1/2,j,k}^{n+1} - E_{x|z+1/2,j,k}^n}{\Delta t} = H_{y|z+1/2,j,k+1/2}^{n+1/2} - H_{y|z+1/2,j,k-1/2}^{n+1/2} - \Delta y \frac{H_{y|z+1/2,j,k}^{n+1/2} - H_{y|z+1/2,j,k-1/2}^{n+1/2}}{\Delta z} - \sigma_{z|z+1/2,j,k}^{n+1/2} \frac{E_{x|z+1/2,j,k}^{n+1} + E_{x|z+1/2,j,k}^n}{2} \quad (4.29)
\]

From Eq. (4.29), the electric field component in \(x\)-direction at the next integer time step is given by:

\[
E_{x|z+1/2,j,k}^{n+1} = \frac{1}{\Delta t} \left( \frac{\epsilon_0 \sigma_{y|z+1/2,j,k}^n}{\Delta t} + \frac{\sigma_{y|z+1/2,j,k}^{n+1/2}}{2} \right) \Delta y \left( H_{y|z+1/2,j,k+1/2}^{n+1/2} - H_{y|z+1/2,j,k-1/2}^{n+1/2} \right) - \frac{1}{\Delta t} \left( \frac{\epsilon_0 \sigma_{y|z+1/2,j,k}^n}{\Delta t} + \frac{\sigma_{y|z+1/2,j,k}^{n+1/2}}{2} \right) \Delta z \left( H_{y|z+1/2,j,k+1/2}^{n+1/2} - H_{y|z+1/2,j,k-1/2}^{n+1/2} \right) + \frac{1}{\Delta t} \left( \frac{\epsilon_0 \sigma_{y|z+1/2,j,k}^n}{\Delta t} + \frac{\sigma_{y|z+1/2,j,k}^{n+1/2}}{2} \right) E_{x|z+1/2,j,k}^n \quad (4.30)
\]

By applying the same procedure, the equations for the electric components in \(y\)- and \(z\)-direction are obtained:

\[
E_{y|z+1/2,j,k}^{n+1} = \frac{1}{\Delta t} \left( \frac{\epsilon_0 \sigma_{x|z+1/2,j,k}^n}{\Delta t} + \frac{\sigma_{x|z+1/2,j,k}^{n+1/2}}{2} \right) \Delta z \left( H_{x|z+1/2,j,k+1/2}^{n+1/2} - H_{x|z+1/2,j,k-1/2}^{n+1/2} \right) - \frac{1}{\Delta t} \left( \frac{\epsilon_0 \sigma_{x|z+1/2,j,k}^n}{\Delta t} + \frac{\sigma_{x|z+1/2,j,k}^{n+1/2}}{2} \right) \Delta x \left( H_{x|z+1/2,j,k+1/2}^{n+1/2} - H_{x|z+1/2,j,k-1/2}^{n+1/2} \right) + \frac{1}{\Delta t} \left( \frac{\epsilon_0 \sigma_{x|z+1/2,j,k}^n}{\Delta t} + \frac{\sigma_{x|z+1/2,j,k}^{n+1/2}}{2} \right) E_{y|z+1/2,j,k}^n \quad (4.31)
\]
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\[ E_{z|i,j,k+1/2}^{n+1} = \frac{1}{\left( \epsilon_0 \epsilon_r |i,j,k+1/2 \Delta t \right)} \left( H_{y|i+1/2,j,k+1/2}^{n+1/2} - H_{y|i-1/2,j,k+1/2}^{n+1/2} \right) \Delta x - \frac{1}{\left( \epsilon_0 \epsilon_r |i,j,k+1/2 \Delta t \right)} \left( H_{x|i,j+1/2,k+1/2}^{n+1/2} - H_{x|i,j-1/2,k+1/2}^{n+1/2} \right) \Delta y + \frac{\epsilon_0 \epsilon_r |i,j,k+1/2 \Delta t}{\epsilon_0 \epsilon_r |i,j,k+1/2 \Delta t} \frac{\sigma |i,j,k+1/2}{2} E_{z|i,j,k+1/2}^{n} \]  

(4.32)

The set of equations given by Eqs. (4.24)-(4.26) and (4.30)-(4.32) define FDTD algorithm. This set of equations connects the electric and magnetic components within the Yee cell for different time steps. In order to calculate the electric and magnetic components, it is necessary to the know relative dielectric permittivity and conductivity of the materials that compose the simulated structure. Since, the relative dielectric permittivity and conductivity are connected to the complex refractive index of the material (Eq. (2.37)), FDTD solvers usually require only the complex refractive index to define the optical properties of the materials. To simplify the FDTD calculations, the optical properties can be preloaded into the computer memory.

For the wide band simulations, the optical properties are analytically fitted so that the computation is efficient [148, 161]. In this study, the experimentally measured optical properties of all materials are fitted for two separate wavelength regions 300-600 nm and 600-1100 nm in order to minimize the fitting error. The analytical fitting of the optical properties is done by an FDTD solver.

The accuracy and stability of the FDTD method depend on the discretization steps in spatial and time domain. While spatial steps have larger influence on the accuracy of the simulation, the time steps are more related to its stability. In order to determine the optimal spatial steps to satisfy the required accuracy of the simulation, the optical properties of the materials and the geometrical properties of the simulated structure have to be taken into account. For bulk materials, the spatial steps are typically determined as a fraction of the wavelength of the light within the material. However, for very thin films, the spatial steps have to be defined as a fraction of the film thickness. Consequently, different spatial steps are required along the simulated solar cell. After the spatial steps are defined, the time step is limited by Courant-Friedrich-Lewy stability criterion [160]:

\[ \Delta t \leq \frac{\epsilon_r |i,j,k|^{\text{min}}}{c \sqrt{(\Delta x)^{-2} + (\Delta y)^{-2} + (\Delta z)^{-2}}} \]  

(4.33)

If the time step is larger than the value defined by Eq. (4.33), the simulation is not stable. Usually, the simulation time steps are defined as a percentage of Courant-Friedrich-Lewy stability criterion.

Quantum efficiency and short circuit current calculations. The outputs of the FDTD simulations are time averaged spatial distribution of electric and magnetic field components. To determine the properties of solar cells such as quantum efficiency and short circuit current, the assumptions defined in Sec. 2.2.1 are used. Consequently, only the charge carriers generated in the i-layer of the solar cell contribute to the
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solar cell current. To determine the quantum efficiency of a solar cell, it has to be taken into account that the electric field components are not obtained at exactly the same position within the Yee cell. Therefore, contributions to the quantum efficiency for each electric field component have to be calculated separately. To calculate the separate components of the quantum efficiency, Eqs. (2.4), (2.8) and (2.11) are used. The quantum efficiency that results from the electric field component in $x$-direction is given by:

$$QE_x(\lambda) = \frac{2\pi\epsilon_0 c \Delta x \Delta y \Delta z}{\lambda P_{in}} \sum_{i,j,k \in i-layer} \eta_{i+1/2,j,k} \cdot |E_x|_{i+1/2,j,k}^2$$ (4.34)

Equation (4.34) assumes that the spatial step in each direction is uniform. For the non-uniform settings, the spatial steps have to be calculated within the sum for all adjacent points. Expressions for the quantum efficiencies that correspond to the electric fields in $y$- and $z$-direction are analogous:

$$QE_y(\lambda) = \frac{2\pi\epsilon_0 c \Delta x \Delta y \Delta z}{\lambda P_{in}} \sum_{i,j,k \in i-layer} \eta_{i,j+1/2,k} \cdot |E_y|_{i,j+1/2,k}^2$$ (4.35)

$$QE_z(\lambda) = \frac{2\pi\epsilon_0 c \Delta x \Delta y \Delta z}{\lambda P_{in}} \sum_{i,j,k \in i-layer} \eta_{i,j,k+1/2} \cdot |E_z|_{i,j,k+1/2}^2$$ (4.36)

In the end, separate contributions have to be summed up:

$$QE(\lambda) = QE_x(\lambda) + QE_y(\lambda) + QE_z(\lambda)$$ (4.37)

The FDTD simulation of a solar cell in superstrate configuration requires that the glass substrate is taken into account. However, due to the fact that the FDTD algorithm assumes coherent light propagation [160], it is not possible to simulate the complete glass substrate. The interference effects in the glass substrate will have a significant effect on the simulated performances of the solar cell. The accurate description of the glass substrate is demonstrated on the example of a flat solar cell (Fig. 4.25).

Figure 4.25a depicts the cross section of the superstrate configuration solar cell as represented in the FDTD solver. In this case, the glass substrate is described by a semi-infinite layer, and the light source is placed within. Direct output of this simulation is the reflectivity ($R_{sim}$) and electric field components from which the total quantum efficiency is calculated (Eqs. (4.34)-(4.37)). To obtain the correct results, the interface between air and the glass substrate has to be taken into account. This is depicted in Fig. 4.25b. For this purpose, the results obtained from the FDTD simulations are combined with the non-interference transfer matrix method (Sec. 2.3.2).

By determining the reflectivity and transmission of the air/glass interface and assuming multiple reflections within the glass substrate, the total quantum efficiency of the superstrate solar cell is given by:

$$QE_{tot}(\lambda) = \frac{T_{int}}{1 - R_{int}R_{sim}}QE(\lambda)$$ (4.38)

which is similar to the approach used to describe the glass substrate for the transparent photodetector (Sec. 2.4). The air/glass interface also has to be taken into account...
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Figure 4.25: (a) Standard FDTD simulation setup with light source within the glass substrate and (b) simulation model developed to account for light source outside the glass substrate.

when determining the total reflectivity of the solar cell. According to non-interference transfer matrix method, the total reflectivity of the solar cell is given by:

$$R_{tot} = R_{int} + \frac{T_{int}^2 R_{sim}}{1 - R_{int} R_{sim}}$$  \hspace{1cm} (4.39)

After the total quantum efficiency is determined, the short circuit current density is calculated by:

$$J_{sc} = \frac{q \Delta \lambda}{\hbar c} \sum_{\lambda} \lambda \cdot AM1.5 (\lambda) \cdot QE_{tot} (\lambda)$$  \hspace{1cm} (4.40)

where it is assumed that the wavelength step of the FDTD simulation is uniform, and that sun spectrum is represented by AM 1.5 standard.

**Comparison of FDTD and analytical methods.** The analytical methods shown in Sec. 2.3.2 can only be used for the optoelectronic devices with flat interfaces. Therefore, to compare the FDTD approach and analytical methods, a-Si:H and µc-Si:H solar cells with flat interfaces are investigated. A cross section of the flat solar cell is already shown in Fig. 4.25.

For a flat a-Si:H solar cell, the front TCO is assumed to be SnO$_2$:F with a thickness of 420 nm. Furthermore, it is assumed that the a-Si:H solar cell consists of 10 nm p-layer, 300 nm i-layer and 10 nm n-layer to match typical a-Si solar cells. The buffer TCO layer is ZnO:Al with a thickness of 100 nm, and the back reflector is silver. The optical data of silver are taken from the literature [65]. For a µc-Si:H solar cell, the front TCO is assumed to be ZnO:Al with a thickness of 500 nm. The thicknesses of the p-, i- and n-layer are 25 nm, 1000 nm and 25 nm, respectively. Again, ZnO:Al is used for buffer layer and silver for the metal back reflector. The thickness of the buffer layer is 80 nm in this case.
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Figure 4.26: (a) Quantum efficiency and (b) reflectivity of a flat a-Si:H solar cell obtained by FDTD simulations and analytical models.

For the FDTD simulations, the spatial step in $z$-direction is non-uniform in order to accurately describe the thin layers. In the interface regions (p-layer, n-layer and buffer layer), the spatial step is 2 nm, while in the bulk regions (front TCO and i-layer) the step is not larger than 7 nm. Due to the flat interfaces, the spatial steps in $x$- and $y$-direction are set to be uniform with 20 nm steps. The time step is set to be 0.85 of the maximum value determined by Courant-Friedrich-Lewy stability criterion (Eq. (4.33)). The wavelength step is 20 nm for wavelengths in range of 300-400 nm and 10 nm otherwise. The simulation for the a-Si:H solar cell is conducted for wavelengths ranging from 300 nm to 800 nm, while for the $\mu$c-Si:H solar cell the range is from 300 nm to 1100 nm. The analytical modeling is achieved by combining the interference and non-interference transfer matrix method. The light propagation through the glass substrate is described as incoherent, while in the other solar cell layers coherent light propagation is assumed. Furthermore, a second model is developed where the light propagation within the i-layer is non-coherent. The wavelength step for the analytical models is 1 nm, and the wavelength regions are the same as for the FDTD simulations.

Figure 4.26 depicts the quantum efficiency and reflectivity of a flat a-Si:H solar cell. An excellent agreement is observed for the results obtained by the FDTD simulation and analytical model with coherent light propagation in the i-layer. The quantum efficiency (Fig. 4.26a) exhibits fringes which appear due to the interference effects in different layers of the solar cell. For shorter wavelengths, the absorption coefficient of the a-Si:H (Fig. 2.2a) is high. Consequently, the light gets absorbed in the front of the solar cell and does not reach the back contact. For this wavelength region, the fringes appear due to the interference effects within the front TCO layer. On the other hand, for longer wavelengths, the absorption coefficient of the a-Si:H (Fig. 2.2a) is low, and the light reaches the back contact. Consequently, the interference fringes for longer wavelengths are influenced by interference effects in the i-layer. This is confirmed by the analytical model where the light propagation in the i-layer is assumed to be non-coherent. In this case, the quantum efficiency exhibits fringes only for shorter wavelengths. The reflectivity of the flat a-Si:H solar cell for different modeling approaches is shown in Fig. 4.26b. Again, a good agreement is observed between the FDTD method and analytical approach with coherent i-layer. The reflectivity curves also exhibit interference fringes. The analytical method with incoherent i-
layer exhibits fringes only shorter wavelengths. In the end, the short circuit current density is calculated for all approaches. Independently of the method, the short circuit current density is 12.5 mA/cm². Consequently, the appearance of interference fringes for longer wavelengths has no influence on the short circuit current of the solar cell.

The quantum efficiency and reflectivity of a flat $\mu c$-Si:H solar cell obtained by the FDTD simulations and analytical approaches are shown in Fig. 4.27. Again, excellent agreement is observed between the FDTD simulations and analytical approach with coherent i-layer. The appearance of fringes in the quantum efficiency curves (Fig. 4.27a) is again influenced by the front TCO and i-layer, which is confirmed by the analytical model with non-coherent i-layer. The reflectivity curves (Fig. 4.27b) exhibit similar trends. For the flat $\mu c$-Si:H solar cell, the number of fringes for longer wavelengths is larger than for the flat a-Si:H solar cell, since the thickness of the i-layer is larger. The calculated short circuit current density of the flat $\mu c$-Si:H solar cell is 14.9 mA/cm² independently of the method used.

The FDTD simulations can be used not only to determine the quantum efficiency and reflectivity of the solar cells, but also to investigate the light propagation within the solar cell and absorption in the individual layers. The light propagation within the solar cell can be visualized by using the electric field intensity ($|E|^2 = |E_x|_{i,j,k}^2 + |E_y|_{i,j,k}^2 + |E_z|_{i,j,k}^2$) or the power loss profile:

$$Q = \frac{2\pi\epsilon_0 c}{\lambda} \eta_{i,j,k} \kappa_{i,j,k} \cdot \left(|E_x|_{i,j,k}^2 + |E_y|_{i,j,k}^2 + |E_z|_{i,j,k}^2\right)$$

(4.41)

where the components of the electric field are interpolated to the origin position of the Yee cell ($i,j,k$). In general, the electric field and power loss maps are determined for an input wave with electric field amplitude of 1 V/m. The calculated maps for the flat a-Si:H solar cell are shown in Fig. 4.28.

Figure 4.28a exhibits the electric field map of the flat a-Si:H solar cell for a wavelength of 400 nm. It can be observed the light does not reach the back reflector and that within the front TCO layer a standing wave is formed. The power loss map (Fig. 4.28b) illustrates the absorption within the solar cell. Although the electric field is high within the front TCO layer, due to the low absorption coefficient (Fig. 2.2b) only small amount of light is absorbed in this layer. From the power loss map, it can
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Figure 4.28: (a) Simulated electric field map and (b) power loss map of the flat a-Si:H solar cell for a wavelength of 400 nm.

Figure 4.29: Simulated power loss maps of the flat (a) a-Si:H and (b) µc-Si:H solar cell for a wavelength of 690 nm.

be observed that for short wavelengths most of the light is absorbed in the front of the solar cell. For short wavelengths, the maps obtained for the flat µc-Si:H solar cell exhibit same trends.

Figure 4.29 depicts the power loss maps of the flat a-Si:H (Fig. 4.29a) and µc-Si:H (Fig. 4.29b) solar cell for a wavelength of 690 nm. In this case, the light reaches the back contact for both solar cells, and standing wave pattern can be observed. The number of standing wave nodes depends on the thickness of the i-layer. Therefore, the µc-Si:H solar cell exhibits more standing wave nodes than the a-Si:H solar cell.

The absorption in the individual layers of the simulated flat solar cells is shown in Fig. 4.30. By determining the absorption in the individual layers, the losses in the solar cell can be identified. Figure 4.30a depicts the losses and quantum efficiency for the flat a-Si:H solar cell. For short wavelengths, the reflection losses are low, but the losses in the front TCO and p-layer are high. For the longer wavelengths, the reflection losses are high since a-Si:H absorbs only small amount of light. The losses in the back contact represent losses in the n-layer, TCO buffer layer and the metal back reflector. The small back contact losses are influenced by the flat interface geometry.

The losses and quantum efficiency of the flat µc-Si:H solar cell are shown in
4.3 Numerical modeling of electromagnetic wave propagation

Figure 4.30: Simulated absorption in the individual layers for the flat (a) a-Si:H and (b) $\mu$c-Si:H solar cell.

Fig. 4.30b. Similar behavior as for the flat a-Si:H solar cell is observed for wavelengths in the range of 300-800 nm. For wavelengths larger than 800 nm, the front TCO exhibits increased absorption since its absorption coefficient increases (Fig. 2.2b). The back contact losses for the flat $\mu$c-Si:H solar cell are also small.

The presented results demonstrate that the FDTD simulations are accurate and comparable to the theoretical results. Furthermore, the FDTD simulations allow for a detailed investigation of the electromagnetic wave propagation and identification of the absorption regions within the solar cell. Finally, by analyzing the absorption in the individual layers, it is possible to determine how to reduce the losses and maximize the quantum efficiency of the solar cells.
4. Silicon thin-film solar cells
Chapter 5

Influence of back contact on optical losses in silicon thin-film solar cells

Silicon thin-film solar cells with both contacts textured can exhibit enhanced light trapping compared to solar cells with only one textured contact [95, 105, 145]. To achieve enhanced light trapping, it is necessary that the front and back contact textures efficiently confine the light within the absorber layer of the solar cell. However, to create the optimal light trapping scheme, a trade-offs for both front and back contact of the solar cell have to be taken into account.

The front contact textures should be optimized to reduce the reflection losses and to efficiently scatter/diffract the light that enters the solar cell. The reflection losses are significantly decreased if the surface textures are smaller than the wavelength of the incoming light [162]. These textures are able to improve the incoupling, but not the scattering/diffraction of the light. By increasing the feature size, the scattering/diffraction of the light is enhanced, but the light incoupling is reduced. The back contact textures should be optimized to reduce absorption losses in the metal back reflector and to scatter/diffract the light that is reflected. Reducing the back contact roughness decreases not only the absorption losses in the back metal reflector, but also scattering/diffraction [89, 105]. However, if the back contact roughness is too large, the absorption in the metal back reflector increases, and the quantum efficiency drops [67].

In general, the optimal surface textures for the front and back contact of the solar cell are different [76, 163]. However, separate optimization of the front and back contact surface textures is difficult to achieve. During the deposition of the solar cell on a textured substrate, surface textures of the substrate propagate through solar cells layers and influence the textures of the other contact. Therefore, in a typical fabrication process of the silicon thin-film solar cells, textures of only one contact can be optimized.

For solar cells in substrate configuration, the textures of the back contact are optimized, while the front contact textures are determined by the back contact morphology and deposition conditions of the solar cell layers. Consequently, the reflection losses of solar cells in substrate configuration are influenced by the back contact textures. For the solar cells in superstrate configuration, the situation is vice versa. The textures of the front contact are optimized, while the back contact morphology and losses are determined by the front contact morphology and deposition conditions of the solar cell layers. To further optimize silicon thin-film solar cells, it is necessary to
determine how surface textures, that are optimized for the front/back contact of the solar cell, influence the light trapping properties of the other contact.

In this chapter, the back contact losses in silicon thin-film solar cells in superstrate configuration are studied. In the first part of the study, optical simulations are used to investigate the optical behavior of the metal reflectors depending on the surface textures and adjacent dielectric material. The influence of the back contact on the optical losses in a-Si solar cells is investigated experimentally and by optical simulations. Furthermore, the optical simulations are used to model and explain the experimental results from the literature for µc-Si solar cells [123]. Parts of this chapter are based on previously published papers [66, 164].

5.1 Metal back reflectors

The back reflector of silicon thin-film solar cells plays a key role in efficient light trapping. Due to the small thickness of silicon thin-film solar cells and low absorption coefficients of silicon materials for longer wavelengths (Fig. 2.2a), light is able to reach the back reflector. The main purpose of the back reflector is to reflect light back into the absorber layer of the solar cell. However, part of the light that reaches the back reflector gets absorbed there. Furthermore, not all the light that gets reflected by the back reflector is absorbed in the absorber layer. A certain amount of light exits the solar cell and increases the reflection losses.

The optical behavior of metals can be explained using the Drude model. This model assumes that the charge carriers in the metal behave like a quasi-free electron gas [46, 165]. At the same time, interactions between electrons, interband transitions and lattice potential are neglected [46, 165]. When the light is incident on the flat metal surface, the electron gas gets displaced under the influence of the electric field component of the electromagnetic wave. Due to the gas displacement, an internal Coulomb interaction is formed between the gas and ion lattice of the metal, which compensates the external electric field. Consequently, the light cannot penetrate the metal and gets reflected. However, since the conductivity of metals is limited, the compensation of the external field can be achieved only for a certain range of wavelengths/frequencies of the incoming light.

Based on the Drude model [46, 165], the complex refractive index of metals is given by:

\[
N^2 = 1 - \frac{\omega_p^2}{\omega^2 + i\Gamma \omega} \tag{5.1}
\]

where \( \omega \) is the frequency of the incoming light, \( \omega_p \) is the plasma frequency of the electron gas, and \( \Gamma \) is the collision or damping frequency. The plasma frequency is a frequency at which the electron gas achieves resonant oscillations, while the collision frequency represents the average number of free carrier collisions per unit of time. If the collision frequency is high, the electron gas oscillations are damped, and the reflectivity of the metal is low.

To demonstrate basic optical properties of metal reflectors, examples of silver and aluminum are used. According to the Drude model, the plasma frequency of silver is \( 2.18 \cdot 10^{15} \) Hz, while its damping frequency is \( 4.35 \cdot 10^{12} \) Hz [166]. For aluminum, the plasma frequency is \( 3.57 \cdot 10^{15} \) Hz, and the damping frequency is \( 19.79 \cdot 10^{12} \) Hz [166]. By using Fresnel's coefficients (Sec. 2.3.1) and the complex refractive index of
absorption wavelength (nm) Photon energy (eV)
(a) (b)

Reflectivity wavelength (nm) Photon energy (eV)
5 10 15 20
0.0 0.2 0.4 0.6 0.8 1.0
1100 300

Absorption wavelength (nm) Photon energy (eV)
5 10 15 20
10^{-3} 10^{-2} 10^{-1} 100
1100 300

Ag Al

5.1 Metal back reflectors

Figure 5.1: (a) Reflectivity and (b) absorption of flat silver and aluminum reflectors according to the Drude model.

the metal (Eq. 5.1), the reflectivity of the flat silver and aluminum reflector can be calculated. To determine the absorption of the flat silver and aluminum reflectors, the simple analytical approach demonstrated in Sec. 2.2.1 is used. According to this approach, the absorption in the metal reflector \( A_{\text{met}} \) is given by:

\[
A_{\text{met}} = (1 - R_{\text{met}}) \cdot (1 - \exp (-\alpha_{\text{met}} \cdot d_{\text{met}}))
\]

where \( R_{\text{met}} \) is the reflectivity of the metal reflector, \( \alpha_{\text{met}} \) is the absorption coefficient of the metal, and \( d_{\text{met}} \) is the thickness of the metal reflector (\( d_{\text{met}} = 1 \mu m \)). The absorption coefficient is obtained by combining Eqs. (2.2), (2.3) and (5.1).

Figure 5.1 depicts the reflectivity (Fig. 5.1a) and absorption (Fig. 5.1b) of the flat silver and aluminum reflectors determined using the Drude model. From Fig. 5.1a, it can be observed that the reflectivity is high if the wavelength of the incoming light is larger than the plasma wavelength. For silver the plasma wavelength is close to 138 nm, and for aluminum is close to 84 nm [166]. In this region, the oscillation frequency of the external electric field is low, and it is compensated by the electron gas [46, 165]. For wavelengths that are smaller than the plasma wavelength, the reflectivity of the metal is low. Now, the oscillation frequency of the external field is high, and the electron gas is not able to compensate it. In this region, the metal behaves like a dielectric, and light is able to penetrate inside [46]. For wavelengths much smaller than the plasma wavelength (x-ray domain), the metal becomes transparent [165]. For wavelengths close to the plasma wavelength, a resonant absorption in the metal is achieved [46, 165], which is shown in Fig. 5.1b.

The resonant oscillations of the electron gas can be excited inside the metal (bulk plasmons), at the surface between the metal and the adjacent dielectric (surface plasmons) or in a small metallic nanostructure (localized plasmons) [46]. As shown in Fig. 5.1, bulk plasmons define the wavelength region in which metals exhibit high reflectivity. The surface plasmons are responsible for coupling of the light into surface plasmon polaritons, which then travel along the metal/dielectric surface [46]. Finally, the localized plasmons are non-propagating electron gas oscillations, which can lead to enhanced scattering of the light [46]. In recent years, the plasmonic effects have been widely investigated in order to develop plasmonic metal back contacts for the
5. Influence of back contact on optical losses in silicon thin-film solar cells

The interaction of light with a metal depends on the surface textures of the metal and the optical properties of the adjacent dielectric. For simple geometries such as spheres or ellipsoids, Mie theory is sufficient to model the scattering and absorption of the metal nanoparticles [46]. However, for more complex structures, numerical methods are required to solve Maxwell’s equations. In this section, the absorption of metal reflectors embedded in a dielectric material is investigated for different surface textures. Furthermore, the influence of the TCO buffer layer (Sec. 4.2.1) on the absorption in metal reflectors is also studied.

Textured metal reflectors. The investigation of textured metal reflectors is focused on silver and aluminum, since these materials are widely used as back contact reflectors in silicon thin-film solar cells [32, 66–68, 89, 95–97, 101, 105–111]. To determine the optical behavior of these reflectors, FDTD simulations have been used. The cross sections of the simulated structures are shown in Fig. 5.2. Figure 5.2a represents a semi-infinite metal reflector with a flat interface, while Fig. 5.2b represents a semi-infinite metal reflector with a pyramid texture.

To simplify the investigation, the adjacent dielectric is represented by a nonabsorbing material with a constant refractive index. Using this approximation, air is represented by a refractive index of 1, ZnO is described by a refractive index of 2 and silicon by a refractive index of 4. For silver and aluminum reflectors, the experimentally measured optical data are taken from the literature [65]. The flat structure is used to compare optical properties of silver and aluminum with the Drude model. On the other hand, the textured metal reflectors are used to demonstrate plasmonic effects. For the textured metal reflector, the textures are represented by square base pyramids in periodic arrangement. The periodic surface textures can be represented by a unit cell, which provides all needed information. In order to determine the absorption of metal reflectors with periodic textures, it is necessary to simulate a single unit cell (Fig. 5.2b).

For the FDTD simulations, the light source is placed within the dielectric. The simulations are carried out for wavelengths from 300 to 1100 nm with step of 5 nm. The wavelength range is chosen to match the absorption spectrum of silicon materials.
5.1 Metal back reflectors

The absorption of the flat silver and aluminum reflector is shown in Fig. 5.3. Although the plasma wavelength of silver is 138 nm, the silver reflector exhibits strong absorption peak around 310 nm (Fig. 5.3a). This absorption peak appears due to the interband absorption in the silver [175], which is neglected in the Drude model. The absorption of the flat silver reflector is minimized for wavelengths longer than 400 nm. By increasing the refractive index of the dielectric material, the absorption of the silver reflector changes slightly (Fig. 5.3a). For dielectric materials with large refractive indices, the absorption becomes larger for longer wavelengths.

The absorption of the flat aluminum reflector is shown in Fig. 5.3b. It can be observed that an absorption peak appears around 800 nm. This is again influenced by interband absorption in aluminum [176]. The absorption of the aluminum reflector is also increasing for larger values of refractive index of the dielectric material. Figure 5.3 also shows that the silver reflector is better than aluminum, which is influenced by its damping frequency [166].

To investigate textured metal reflectors, different dimensions for the period and height of the square base pyramid (Fig. 5.2b) are used. Localized plasmonic effects can be observed for the size of features that are smaller than 100 nm [46]. To observe plasmonic effects in textured metal reflectors, the period of the pyramid is set to 50 nm and the height to 15 nm. On the other hand, the average feature size of light trapping structures is larger than 400 nm (Sec. 4.2.2). Therefore, to investigate the behavior of the metal reflectors in this domain, the period of the pyramid is set to 500 nm and its height to 150 nm.

Figure 5.4 depicts the absorption of textured silver and aluminum reflector for the period of pyramid of 50 nm and height of 15 nm. The absorption of the textured silver reflector (Fig. 5.4a) exhibits plasmonic absorption peaks [46]. By reducing the refractive index of the dielectric, the plasmon resonances shift to shorter wavelengths. For nonabsorbing silicon material ($N = 4$), the plasmon resonance is close to 800 nm. The plasmon resonance is shifted to 450 nm for ZnO ($N = 2$) and 345 nm for air ($N = 1$). For the aluminum reflector (Fig. 5.4b), plasmonic absorption occurs only

![Figure 5.3: Absorption of flat (a) silver and (b) aluminum reflector. The absorption is shown for different refractive indices of the adjacent dielectric material.](image-url)
5. Influence of back contact on optical losses in silicon thin-film solar cells

Figure 5.4: Absorption of textured (a) silver and (b) aluminum reflector for period/height of the pyramid of 50/15 nm.

Figure 5.5: Absorption of textured (a) silver and (b) aluminum reflector for period/height of the pyramid of 500/150 nm.

for the silicon dielectric. By reducing the refractive index, the plasmonic resonance is shifted below 300 nm.

Figure 5.5 depicts the absorption of the silver and aluminum reflector for the pyramid period/height of 500/150 nm. The dimensions of the structure are outside the domain in which localized plasmonics can be excited [46], and the absorption peaks are not related to the plasmonic effects. The absorption of the silver reflector is shown in Fig. 5.5a. For ZnO dielectric, the silver reflector exhibits an absorption peak at wavelength longer than 1100 nm. By changing the dielectric to air, the absorption peak is shifted to 600 nm. Same behavior is observed for the textured aluminum reflector (Fig. 5.5b). Although the optical constants of silver and aluminum are different, the wavelengths of absorption peaks for the aluminum reflector are comparable to that of silver (Fig. 5.5a). Therefore, these absorption peaks can be contributed to the geometry of the texture.

Influence of TCO buffer layer. As stated in Sec. 4.2.1, the back contact of silicon thin-film solar cell can be either a back reflector or a back reflector with a
TCO buffer layer. Since silver and aluminum exhibit excellent electrical properties, the TCO buffer layer is not needed to improve the charge collection as for the white paint reflector. However, the TCO buffer layer can have a significant influence on the absorption losses in the metal reflector.

To investigate the influence of the buffer layer on the absorption in the metal reflector, only the back contact of a solar cell is investigated. It is assumed that the back contact consists of a silicon material, TCO buffer layer and textured metal reflector (Fig. 5.6). To simplify the investigation the silicon material is described by reflective index of 4. As TCO buffer layer, air \((N = 1)\) and ZnO \((N = 4)\) are used. The thickness of the TCO buffer layer is set to 100 nm (Sec. 4.2.1). The aluminum and silver reflectors are described by the measured optical data [65].

Figure 5.6 schematically depicts the cross sections of the investigated structures. The metal reflectors with flat interfaces (Fig. 5.6a) are investigated to determine the influence of the buffer layer when plasmonic and geometrical effects are not present. For the textured metal reflectors, a pyramid texture is used (Fig. 5.6b). In this investigation, it is assumed that the pyramid texture propagates unchanged through the buffer layer.

The absorption of the flat silver and aluminum reflector is shown in Fig. 5.7. As a reference, the case without TCO buffer layer is also depicted. The absorption of the silver reflector (Fig. 5.7a) is similar to the case when the silver reflector is embedded in the dielectric material (Fig. 5.3a). However, due to the TCO buffer layer, a Fabry-Perot resonator is formed between the silicon and silver, and additional absorption peak can be observed. The absorption of the aluminum reflector (Fig. 5.7b) also exhibits Fabry-Perot resonances at almost the same wavelength.

The absorptions of the silver and aluminum reflectors with the buffer layer for a pyramid texture with period/height of 50/15 nm are shown in Fig. 5.8. For the silver reflector (Fig. 5.8a), it can be observed that by introducing the buffer layer, the plasmonic resonances are shifted to shorter wavelengths, which is a similar effect as for the silver reflector embedded in the dielectric (Fig. 5.4a). For the aluminum reflector (Fig. 5.8b), the plasmonic absorption peaks are not present when the buffer layer is introduced. However, an additional peak can be observed. This peak can be contributed to the Fabry-Perot resonator, since it is located at the same wavelength.
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Figure 5.7: Absorption of flat (a) silver and (b) aluminum reflector. The absorption is shown for different refractive indices of the TCO buffer layer.

Figure 5.8: Absorption of textured (a) silver and (b) aluminum reflector with buffer layer for period/height of the pyramid of 50/15 nm.

as for the flat case (Fig. 5.7b). Compared to the flat case (Fig. 5.7b), the absorption of the aluminum reflector is increased since the pyramid texture enhances incoupling of the light into the back reflector.

Figure 5.9 shows the absorption of the silver and aluminum reflector with buffer layer for a pyramid texture with period 500 nm and height 150 nm. The geometry effects are suppressed both for the silver (Fig. 5.9a) and aluminum reflector (Fig. 5.9b). Since the refractive index of the buffer layer is smaller than that of silicon, there is a reflection at the silicon/buffer layer interface, which reduces the amount of light that reaches the metal reflector. The influence of the buffer layer is more pronounced for the aluminum reflector (Fig. 5.9b) than for silver (Fig. 5.9a), due to their optical properties and different damping frequencies [65, 166].

Perfect absorber. Previous results show that the influence of the dielectric buffer layer depends on texture dimensions. For small features, due to the lower refractive index of the buffer layer, the plasmonic resonances are shifted to shorter wavelengths. On the other hand, for larger features, the buffer layer acts as a reflection coating
and reduces the amount of light that reaches the back reflector. In order to further investigate the influence of the dielectric buffer layer, a case of a perfect absorber is analyzed.

The perfect absorber absorbs all incoming light and exhibits no plasmonic or Fabry-Perot effects. When the buffer layer is not present, the absorption of the perfect absorber is equal to one for all wavelengths. However, when the buffer layer is present, some of the light will be reflected at the silicon/buffer layer interface, and the absorption in the back contact is reduced. Therefore, the absorption in the back contact with perfect absorber depends on the optical properties of the buffer layer and dimensions of surface textures at the interface between the buffer layer and silicon solar cell. The structures simulated in this investigation are shown in Fig. 5.6 where the metal reflector is replaced by a perfect absorber.

The absorption of the perfect absorber for different textures and buffer layer materials is shown in Fig. 5.10. The dashed lines are used to show the case when the
back contact is not textured. For a period/height of the pyramid texture of 50/15 nm (Fig. 5.10a), the absorption is slightly increased compared to the flat case. For shorter wavelengths, the absorption increase is larger. In this wavelength region, the textures are able to improve the light incoupling into the perfect absorber. For longer wavelengths, the textures are small to improve light incoupling, and the absorption is comparable to the flat case. Unlike silver or aluminum (Fig. 5.8), the perfect absorber exhibits no absorption peaks. This confirms that in the case of small features the absorption peaks of silver and aluminum are due to the excitation of the plasmonic and Fabry-Perot resonances.

The absorption of the back contact with a texture period/height of 500/150 nm is shown in Fig. 5.10b. The absorption of the perfect absorber is now smaller than for the flat case. By changing the buffer layer material, shifting of the absorption peaks is observed same as for silver and aluminum (Fig. 5.9). Similar behavior between metals and perfect absorber confirms that these absorption peaks are influenced by the geometry of the texture and not by the excitation of plasmonic resonances. Furthermore, by reducing the refractive index of the buffer layer material, the absorption of the perfect absorber is reduced, which is similar to the aluminum reflector (Fig. 5.9b). Consequently, the perfect absorber can be described as a metal with infinite damping frequency.

5.2 Back contact losses in a-Si:H solar cells

The light trapping in silicon thin-thin film solar cells in superstrate (p-i-n) configuration can be maximized by optimizing the front contact textures and reducing the back contact losses. The front contact textures are controlled by the fabrication process of randomly textured substrates. The back contact losses depend on the back contact morphology and the optical properties of the TCO buffer layer and metal reflector. The back contact morphology is determined by the front contact textures and silicon film formation (Sec. 4.2.3). Therefore, the back contact losses can be tuned by texturing or smoothing the surface of the TCO buffer layer which is deposited on the silicon solar cell [67, 105, 177, 178]. Furthermore, the back contact losses can be controlled by using different materials for the buffer layer and metal reflector [89, 105, 108, 109, 111, 114, 119, 120].

In this study, the back contact losses in a-Si:H superstrate configuration solar cells deposited on randomly textured SnO$_2$:F substrates are investigated. The investigation is achieved experimentally and using FDTD simulations. Schematic cross sections of the investigated a-Si:H solar cells are shown in Fig. 5.11. The investigation is focused on the influence of the TCO buffer layer on the back contact losses. The influence is determined by comparing solar cells with buffer layer (Fig. 5.11a) to solar cells without buffer layer (Fig. 5.11b). The material used for the buffer layer is ZnO:Al, and the investigation is conducted for silver and aluminum reflectors.

5.2.1 Experimental investigation

The fabrication and experimental measurements of a-Si:H solar cells have been done at Malibu GmbH and Co. KG. In the first step, the a-Si:H solar cells are prepared by PECVD process. The solar cells are deposited on glass substrates coated with randomly textured SnO$_2$:F. The randomly textured SnO$_2$:F has been fabricated by
Nippon Sheet Glass company. The area of the substrates is 1.43 m². The total thickness of a-Si:H solar cells is 320 nm, where the p-, i- and n-layer are 10 nm, 300 nm and 10 nm, respectively. The back contacts of the a-Si:H solar cells are composed of silver or aluminum reflectors with and without ZnO:Al buffer layer. The ZnO:Al buffer layer and metal reflectors are deposited by DC magnetron sputtering. The thickness of the ZnO:Al buffer layer is 100 nm. After the deposition of the solar cell layers, laser scribing is used to define the area of the solar cells to 1 cm². In the next step, the current voltage characteristics of the fabricated a-Si:H solar cells (Fig. 5.12) are measured under illumination from an AM 1.5 sun spectrum simulator.

Figure 5.12 depicts the current voltage characteristics and electric parameters of a-Si:H solar cells with different back contact configurations. Furthermore, energy conversion efficiencies are also shown. The lowest short circuit current density is observed for the aluminum back contact without ZnO:Al buffer layer (Fig. 5.12a). However, the fill factor and open circuit voltage are high resulting in a conversion efficiency of 8.6 %. By introducing the buffer layer between the a-Si:H p-i-n solar cell and the aluminum reflector, the short circuit current density increases by 1.2 mA/cm² (Fig. 5.12b). In this case, the fill factor and open circuit voltage are not affected by the ZnO:Al buffer layer. The conversion efficiency is increased to 9.4 %. The solar cell with silver reflector without ZnO:Al buffer layer (Fig. 5.12c) exhibits the smallest fill factor, which is influenced by the highest series and lowest shunt resistance. Due to the low fill factor, the conversion efficiency is only 8.4 %. The short circuit current density of the a-Si:H solar cell with silver reflector and ZnO:Al buffer (Fig. 5.12d) layer is highest. Compared to the solar cells with a-Si/Ag and a-Si/ZnO/Al back contacts, the short circuit current density is increased by 0.7 mA/cm² and 0.5 mA/cm², respectively. Furthermore, the series and shunt resistance are also improved, and the fill factor is comparable to the aluminum reflector solar cells. Consequently, the conversion efficiency is highest with a value of 9.6 %.

For all fabricated solar cells, the series resistance is almost 10 times smaller, while the shunt resistance is at least 10 times larger than the characteristic resistance.
5. Influence of back contact on optical losses in silicon thin-film solar cells

Therefore, the short circuit densities are not influenced by the electrical properties of the solar cells (Sec. 4.1). It can be concluded that the short circuit current densities depend only on the optical properties of the back contacts. To further investigate the optics of the fabricated solar cells, the quantum efficiency and total absorption of the fabricated solar cells are also measured. The total absorption can be determined from measurement of the total reflectivity ($A_{\text{tot}} = 1 - R_{\text{tot}}$). In order to obtain the total reflectivity, an UV-VIS spectrometer with an integrating sphere is used to measure specular and diffused reflectivity of the fabricated solar cells. Finally, the sum of the specular and diffused reflectivity represents the total reflectivity. The quantum efficiency and the total absorption of the fabricated a-Si:H solar cells are shown in Fig. 5.13.

Figure 5.12: Current voltage characteristics and electric parameters of a-Si:H solar cells for (a) a-Si/Al, (b) a-Si/ZnO/Al, (c) a-Si/Ag and (d) a-Si/ZnO/Ag back contact configuration.

Therefore, the short circuit densities are not influenced by the electrical properties of the solar cells (Sec. 4.1). It can be concluded that the short circuit current densities depend only on the optical properties of the back contacts. To further investigate the optics of the fabricated solar cells, the quantum efficiency and total absorption of the fabricated solar cells are also measured. The total absorption can be determined from measurement of the total reflectivity ($A_{\text{tot}} = 1 - R_{\text{tot}}$). In order to obtain the total reflectivity, an UV-VIS spectrometer with an integrating sphere is used to measure specular and diffused reflectivity of the fabricated solar cells. Finally, the sum of the specular and diffused reflectivity represents the total reflectivity. The quantum efficiency and the total absorption of the fabricated a-Si:H solar cells are shown in Fig. 5.13.

Figure 5.13a depicts the measured results for the fabricated a-Si:H solar cells with aluminum reflector with and without ZnO:Al buffer layer. For wavelengths shorter than 500 nm, the incoming light gets absorbed in the front of the solar cells and does not reach the back contact. Consequently, there is no difference in the quantum efficiency and total absorption. For wavelengths longer than 500 nm, the incoming light reaches the back contact, and the quantum efficiencies and total absorption depend on the back contact design. Although the solar cell without ZnO:Al buffer layer exhibits higher total absorption for wavelengths longer than 650 nm, its quantum efficiency is lower compared to the solar cell with buffer layer. Similar trends are also
5.2 Back contact losses in a-Si:H solar cells

Figure 5.13: Quantum efficiency and absorption of fabricated solar cells with and without ZnO:Al buffer layer for (a) aluminum and (b) silver reflector.

observed for the a-Si:H solar cells with silver reflector (Fig. 5.13b).

For the solar cells with silver reflector, the influence of the buffer layer on the quantum efficiency is smaller than for the solar cells with aluminum reflector. This is influenced by the optical properties of silver and aluminum. Since the reflection properties of silver are better than for aluminum, the ZnO:Al buffer layer is more important for the aluminum reflector.

The presented experimental results show that the measured quantum efficiency of the fabricated solar cells cannot be correlated directly to the total absorption of the solar cell. Therefore, it is necessary to determine the absorption in the individual layers of the solar cell. However, such direct measurements are not possible. Consequently, FDTD optical simulations have to be used to investigate the behavior of solar cells for different back contact designs.

5.2.2 Optical model

The first step in computational investigations is to create accurate optical model of the experimentally realized solar cells. Therefore, the optical properties of the materials implemented in the optical simulations have to correspond to the materials used for the fabrication of the solar cells. Furthermore, the textured interfaces of the fabricated solar cells have to be accurately represented in the optical model. This can be achieved by using AFM measurements of the front and back contact of the experimentally realized solar cells [83]. However, these AFM measurements require complicated alining procedure using laser markers [81, 82]. As an alternative, the simulated solar cells structures can be created using only the AFM measurements of the front contact, while the back contact textures are simulated using different models [83, 92, 152]. Although the approaches that implement experimentally measured interfaces are accurate, they are complex and time consuming since the simulated areas range from 2.5 x 2.5 µm² [92, 152] to more than 5.5 x 5.5 µm² [83].

A different approach in creating the solar cell structures for optical simulations is to use periodic surface textures. Previous studies have shown that the randomly textured or quasi-random substrates, such as the artificially created substrates presented in Sec. 4.2.2, can be described as an area-weighted superposition of periodic
5. Influence of back contact on optical losses in silicon thin-film solar cells

substrates with dimensions that correspond to individual substrate features (Figs. 4.9 and 4.13) [75, 179]. However, this approach requires large number of simulations to account for each individual feature. To reduce the number of simulations, in this study it is assumed that the quasi-random substrates can be represented by a periodic substrate with textures that correspond to an area-weighted average feature (Sec. 4.2.2). In Sec. 4.2.2, it is shown that the individual features of randomly textured SnO$_2$:F substrate can be approximated by square base pyramids (Fig. 4.10) and that area-weighted average feature has a period of 400 nm and height of 108 nm. To simplify the geometry of the optical model, the height is rounded up to 110 nm. To obtain complete information of the periodic substrate, only a single unit cell is needed (Fig. 5.14a). To describe the back contact textures, the surface coverage algorithm (Sec. 4.2.3) is used. The direction factor is set to one.

The surface textures of the developed optical model are shown in Fig. 5.14. Figure 5.14a depicts the unit cell and the front contact morphology of the periodic substrate, where the pyramid textures are placed on top of 420 nm thick flat SnO$_2$:F layer (Sec. 4.3.1). The back contact of the developed optical model is shown in Fig. 5.14b. To simulate the morphology of the back contact, the total thickness of the a-Si:H p-i-n solar cell is set to 320 nm based on the experimentally realized solar cells. From Fig. 5.14b it can be observed that the back contact morphology is smoother than the front contact. Furthermore, due to the smoother textures, the local film thickness is increased, which leads to larger average film thickness.

To compare randomly textured SnO$_2$:F (Fig. 4.10a), quasi-random (artificial) (Fig. 4.10b) and periodically textured substrate (Fig. 5.14a), the surface coverage algorithm is used to determine the surface roughness and average i-layer thickness. In this investigation, the nominal film thicknesses of the p- and n-layer are 10 nm, while the nominal thickness of the i-layer is varied. The results are shown in Fig. 5.15

Figure 5.15a depicts the surface roughness as a function of the nominal i-layer thickness. The surface roughness drops as the nominal thickness of the i-layer increases. The drop of roughness depends on the type of the substrate. In Sec. 4.2.2, it is determined that the roughness of the randomly textured SnO$_2$:F is 38.4 nm, while the roughness of the quasi-random substrate is 40.3 nm. The roughness of a
5.2 Back contact losses in a-Si:H solar cells

Figure 5.15: (a) Surface roughness and (b) i-layer thickness gain of textured SnO$_2$:F substrate and its approximations as a function of the nominal i-layer thickness.

periodically textured substrate with square base pyramid texture is given by [79]:

$$ \text{rms}_{sq-pyr} = \frac{H_{pyr}}{3\sqrt{2}} $$  \hspace{1cm} (5.3)

where $H_{pyr}$ is the height of the pyramid texture. For a height of the pyramid of 110 nm, the surface roughness is 25.9 nm. For a nominal thickness of the i-layer of 300 nm, the back contact roughness of the randomly textured SnO$_2$:F is 33 nm, which is a drop of 14 % compared to the front contact. For the quasi-random substrate, the drop of roughness is only 8 %, while the rms roughness of the back contact is 36.9 nm. For the periodically textured substrate, the back contact roughness is 21.2 nm, and the drop is 18 %.

The average thickness of a solar cell layer ($t_{layer-avg}$) is given by [79]:

$$ t_{layer-avg} = \frac{V_{layer}}{A} $$ \hspace{1cm} (5.4)

where $V_{layer}$ is the volume of the layer, and $A$ is the area for which the volume is calculated. Using Eq. (5.4), the average thickness of the p-layer is calculated for different substrates. For the randomly textured SnO$_2$:F, the average thickness of the p-layer is 12.2 nm. The average p-layer thickness for the quasi-random substrate is 11.2 nm and for the periodically textured substrate is 11.4 nm. The increase of the layer thickness can also be described by the thickness gain ($t_{gain}$) [81]:

$$ t_{gain} = \frac{t_{layer-avg} - t_{layer-nom}}{t_{layer-nom}} $$ \hspace{1cm} (5.5)

where $t_{layer-nom}$ is the nominal film thickness. The thickness gain of the i-layer for different substrates is shown in Fig. 5.15b. The thickness gain drops with increasing nominal thickness of the i-layer. For a nominal thickness of the i-layer of 300 nm, the thickness gain for the randomly textured SnO$_2$:F is 13 %, and the average i-layer thickness is 339 nm. For the artificial substrate, the average i-layer thickness is 331.5 nm resulting in the thickness gain of 10.5 %. The thickness gain and average
5. Influence of back contact on optical losses in silicon thin-film solar cells

i-layer thickness for the periodically textured substrate are 10.8 % and 332.4 nm, respectively.

The front and back contact roughness of the periodically textured substrate are smaller than those of the randomly textured and quasi-random substrate. However, the drop of back contact roughness is comparable with the randomly textured substrate. On the other hand, the average thickness of the i-layer for all substrates is almost the same. From the results presented in Fig. 5.15, it can be concluded that the periodically textured substrate can be used to approximate the randomly textured or quasi-random substrates.

5.2.3 Simulation results

After developing the optical model, it is necessary to include the interface morphologies and material properties into the optical simulations. Therefore, periodic pyramid textures and simulated morphologies of the p-, i- and n-layer are implemented into the FDTD solver. Furthermore, it is assumed that the ZnO:Al buffer layer, if present, has negligible influence on the morphology of the back contact. Consequently, the morphology of the ZnO:Al buffer layer is the same as the morphology of the n-layer. The simulation settings have been the same as for the flat simulations (Sec. 4.3.1). The spatial step in x- and y-direction is 8 nm.

From the FDTD simulations, the time averaged power loss maps are obtained. Since wavelengths shorter than 500 nm do not reach the back contact (Sec. 4.3.1), the power loss profiles are determined for a wavelength of 690 nm to show the interaction of light with different back contact configurations (Fig. 5.16). Cross sections of the simulated solar cell structures are shown in Figs. 5.16a and 5.16b. It can be observed that the interface morphology is changing due to the a-Si:H film formation. Figures 5.16c and 5.16d exhibit power loss maps for the aluminum reflector. It can be observed that the light penetrates almost 30 nm inside the aluminum reflector. On the other hand, the light penetrates only 10 nm inside the silver reflector, which is shown in Figs. 5.16e and 5.16f. By comparing the solar cell structures with (Figs. 5.16d and 5.16f) and without (Figs. 5.16c and 5.16e) ZnO:Al buffer layer, it can be observed that the absorption in the i-layer is improved when ZnO:Al buffer layer is present. For the back contact with the buffer layer, more light is reflected back into the i-layer, and the absorption is enhanced. To further investigate the influence of the ZnO:Al buffer layer and metal reflectors on the performance of solar cells, absorption in the individual layers of the simulated solar cells is calculated and shown in Fig. 5.17.

The calculated quantum efficiency and optical losses for solar cells with aluminum reflector are shown in Figs. 5.17a and 5.17b. Same as for the experimental results (Fig. 5.13a), the solar cell without ZnO:Al buffer layer (Fig. 5.17a) exhibits higher total absorption and lower quantum efficiency compared to the solar cell with ZnO:Al buffer layer (Fig. 5.17b). These trends are influenced by the back contact absorption. The solar cell without ZnO:Al buffer layer exhibits higher back contact losses and increased total absorption. Higher back contact losses limit the amount of light that is reflected back into the i-layer, and the quantum efficiency is lower. By introducing the ZnO:Al buffer layer, the reflectivity of the back contact is improved, and more light is being reflected back into the solar cell resulting in an increased quantum efficiency. However, not all the light reflected by the back contact gets absorbed in the i-layer. A part of it exits the solar cell and increases the reflection losses. Consequently,
5.2 Back contact losses in a-Si:H solar cells

Figure 5.16: Cross sections of simulated unit cells (a) without and (b) with ZnO:Al buffer layer. Corresponding power loss maps for (c) a-Si/Al, (d) a-Si/ZnO/Al, (e) a-Si/Ag and (f) a-Si/ZnO/Ag back contact configuration (wavelength of 690 nm).

the total absorption is lower compared to the solar cell without ZnO:Al buffer layer. Similar trends are observed for solar cells with silver reflector (Figs. 5.17c and 5.17d). A comparison of the solar cells with aluminum (Figs. 5.17a and 5.17b) and silver reflector (Figs. 5.17c and 5.17d) shows that the influence of the ZnO:Al buffer layer is more pronounced for the aluminum reflector, which is consistent with the experimental results. Finally, the losses in the front TCO layer and p-layer are independent of the back contact design.

A comparison of the simulated (Fig. 5.17) and experimental results (Fig. 5.13) shows that the simulated reflectivity is higher than the measured one for the complete wavelength range of 300 nm to 800 nm. This is influenced by different factors for short and long wavelengths. For wavelengths shorter than 500 nm, the simulated structures exhibit lower light incoupling compared to the experimentally realized solar cells. The randomly textured substrates are composed of features with different dimensions (Fig. 4.9), where smaller features improve the light incoupling, while the larger features improve the light scattering/diffraction. On the other hand, the simu-
5. Influence of back contact on optical losses in silicon thin-film solar cells

Figure 5.17: Calculated quantum efficiencies and optical losses for (a) a-Si/Al, (b) a-Si/ZnO/Al, (c) a-Si/Ag and (d) a-Si/ZnO/Ag back contact configuration.

lated solar cells are composed of a single periodic texture. Due to its period of 400 nm, this texture is not able to accurately account for the light incoupling that is observed in the experimentally realized solar cells. To overcome this problem, a set of periodic simulations with different periods and height can be used [79]. For wavelengths longer than 500 nm, the simulated reflectivity is larger than the experimental due to the back reflector of the solar cell. When depositing metals on rough surfaces, a porous metal films are formed [180–183]. Consequently, the optical properties of the porous metal films are not equal to those of the bulk metal layers [181–183]. Porous metals tend to absorb more light than bulk layers [181–183]. Since in the simulations the optical properties of bulk metals were used, the reflectivity of the metal reflectors is higher than for the experiment. To overcome this problem and improve the simulation model, the optical properties of porous metal films should be accounted for.

To quantify the trade-off between the back contact losses and quantum efficiencies, the absorptions in the individual layers are converted into current densities (Eq. (4.40)). Furthermore, the simulation results for solar cells with perfect absorber are used as a reference. The results are summarized together with the experimental data in Tab. 5.1.

The simulated short circuit current densities for a-Si/Al, a-Si/Ag, a-Si/ZnO/Al,
5.2 Back contact losses in a-Si:H solar cells

Table 5.1: Simulated short current densities and optical losses of a-Si:H solar cells for different back contact configurations.

<table>
<thead>
<tr>
<th>Back contact configuration</th>
<th>Short circuit current density (mA/cm²)</th>
<th>Simulated optical losses (mA/cm²)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>measured</td>
<td>simulated</td>
</tr>
<tr>
<td>a-Si/PA</td>
<td>–</td>
<td>11.4</td>
</tr>
<tr>
<td>a-Si/Al</td>
<td>13.3</td>
<td>13.9</td>
</tr>
<tr>
<td>a-Si/Ag</td>
<td>14.3</td>
<td>14.8</td>
</tr>
<tr>
<td>a-Si/ZnO/PA</td>
<td>–</td>
<td>12.8</td>
</tr>
<tr>
<td>a-Si/ZnO/Al</td>
<td>14.5</td>
<td>15.1</td>
</tr>
<tr>
<td>a-Si/ZnO/Ag</td>
<td>15.0</td>
<td>15.6</td>
</tr>
</tbody>
</table>

and a-Si/ZnO/Ag back contact show good agreement with the measured results. The simulated current densities are higher by 0.5-0.6 mA/cm², but the trends and differences are the same as for the measured values. To understand the trade-off between the back contact losses and quantum efficiency due to the ZnO:Al buffer layer, a case with a perfect absorber is analyzed. By introducing the ZnO:Al buffer layer, the back contact losses for the perfect absorber drop by 2.6 mA/cm². Consequently, more light is reflected back into the i-layer. The short circuit current density is increased by 1.4 mA/cm², while the rest contributes to the front contact and reflection losses. The behavior of the aluminum reflector is comparable to that of the perfect absorber. Although the back contact losses are much smaller than for the perfect absorber, their drop due to the ZnO:Al buffer layer is the same. Due to the smaller back contact losses, the short current density increases by 1.2 mA/cm² in this case, while the rest is distributed between the front contact and reflection losses. The perfect reflector is not able to nicely model the behavior of the silver reflector. Due to the excellent optical properties, the back contact losses for the silver reflector are further reduced. Due to the small back contact losses, the influence of the ZnO:Al buffer layer is smaller. The drop of the back contact losses is 1.1 mA/cm² in this case. The short circuit current density increases by 0.8 mA/cm², while the front contact losses are increased by 0.3 mA/cm².

The simulation results show that the back contact losses depend on the optical properties of the metal reflector and adjacent dielectric material. By introducing the ZnO:Al buffer layer, the back contact losses are reduced, while the quantum efficiency, reflection and front contact losses are increased. The trade-off between the optical losses and the quantum efficiency also depends on the back contact morphology. As shown in Fig. 5.15a, the roughness of the back contact is reduced with increasing thickness of the i-layer. Furthermore, the lateral size of the back contact features is increased with increasing thickness of the i-layer [81, 82]. Taking these considerations into account, the back contact morphology of a 320 nm thick a-Si:H solar cell would be almost flat if the average front contact feature is smaller than 200 nm [79]. The flat back contact exhibits low absorption losses. However, the drop of the back contact losses will mainly result in an increased reflection and front contact losses, due to poor light trapping properties of the flat back contact. For an average feature size of the front contact larger than 300 nm, the trade-off depends on the ratio between the period and height of the front contact features. If the period is much larger than
5. Influence of back contact on optical losses in silicon thin-film solar cells

![Figure 5.18: Schematic cross section of a μc-Si:H solar cell on etched ZnO:Al substrate (a) with and (b) without ZnO:Al buffer layer.](image)

The height, the back contact again will be almost flat. On the other hand, if the height is much larger than the period, the roughness of the back contact will be large. Consequently, the back contact losses will be large even when the ZnO:Al buffer layer is present resulting in a low quantum efficiency. Therefore, to design the optimal front contact textures it is necessary to take into account their influence on the back contact losses.

5.3 Back contact losses in μc-Si:H solar cells

The back contact morphology of μc-Si:H solar cells (Figs. 4.17b and 4.21a) is a superposition of large and small features. The large features are substrate textures that propagate through μc-Si:H solar cell, while the nanofeatures are natural textures that are formed during μc-Si:H film growth. Although the dimensions of the nanofeatures are significantly smaller than the larger surface textures, their influence on the back contact losses cannot be neglected. As shown by the results in Sec. 5.1, the nanofeatures are able to excite the localized plasmonic resonances in the metal reflectors and increase the back contact absorption.

In this study, the trade-off between the back contact losses and the quantum efficiency of μc-Si:H superstrate configuration solar cells is investigated. Figure 5.18 schematically depicts the cross sections of μc-Si:H solar cells deposited on etched ZnO:Al substrate with (Fig. 5.18a) and without (Fig. 5.18b) ZnO:Al buffer layer. Due to the small thickness of the ZnO:Al buffer layer (Fig. 4.7), it can be assumed that the nanofeatures are able to propagate through the ZnO:Al film (Fig. 5.18a). The aim of the study is to determine the influence of the ZnO:Al buffer layer and μc-Si:H natural textures on the back contact losses. The investigation has been conducted for silver and aluminum metal reflectors using FDTD simulations. Experimental results from literature are used as a reference for the silver reflector [123].
5.3 Back contact losses in $\mu$-Si:H solar cells

Figure 5.19: Quantum efficiency of a $\mu$-c-Si:H solar cells on etched ZnO:Al substrate with and without ZnO:Al buffer layer for a silver reflector [123].

5.3.1 Experimental investigation

The influence of a TCO buffer layer on the performance of single junction silicon thin-film solar cells has been systematically studied by Jülich Research Center [89, 105, 123, 184]. The studies have been focused on the experimental investigation of $\mu$-c-Si:H and a-Si:H solar cells prepared on etched ZnO:Al substrates. As the back contact, silver reflectors with and without ZnO:Al buffer layer have been used (Figs. 5.18a and 5.18b). In this investigation, the experimental results from Jülich Research Center are used as a reference [123].

The part of the experimental investigation conducted at Jülich Research Center has been focused on $1\ \mu m$ thick $\mu$-c-Si:H solar cell deposited on etched ZnO:Al substrate [123]. In the first step, a silver reflector is directly deposited on top of the $\mu$-c-Si:H solar cell. After the measurement of the quantum efficiency, the metal reflector is removed by template striping [123]. In the next step, a back contact consisting of an 80 nm thick ZnO:Al buffer layer and silver reflector is deposited by a sputtering process. Using this approach, the back contact morphology is the same for both measurements of the quantum efficiency. Finally, the quantum efficiency is measured for $\mu$-c-Si/ZnO/Ag back contact.

Figure 5.19 depicts experimentally measured quantum efficiencies [123]. For wavelengths shorter that 550 nm, the light does not reach the back contact, and the quantum efficiencies of the solar cells with and without ZnO:Al buffer layer are the same. For wavelengths longer than 550 nm, the quantum efficiency depends on the back contact configuration. In this wavelength range, the solar cell with the ZnO:Al buffer layer exhibits higher quantum efficiency than the solar cell without the buffer layer.

Although $\mu$-c-Si:H solar cells with and without ZnO:Al buffer layer exhibit same trends as a-Si:H solar cells (Fig. 5.13b), the influence of the ZnO:Al buffer layer is much larger in this case. The short circuit current density is increased by 2 mA/cm$^2$ due to the ZnO:Al buffer layer, which is 4 times larger than for the a-Si:H solar cells.

The experimental investigation also reveals that by reducing the refractive index of the buffer layer, the short circuit density can be further increased [123]. Experimental results show that by using silicon dioxide ($\text{SiO}_2$) as a buffer layer material, the short circuit density is increased by 0.3 mA/cm$^2$ compared to the ZnO:Al buffer layer.
5. Influence of back contact on optical losses in silicon thin-film solar cells

5.3.2 Optical model

To develop an optical model of µc-Si:H solar cells deposited on etched ZnO:Al substrate, a periodic approximation is used (Sec. 5.2.2). As shown in Sec. 4.2.2, the crater textures of etched ZnO:Al can be described by inverted cones with fixed diameter to depth ratio (Figs. 4.14 and 4.15). To create periodic approximation of the etched ZnO:Al substrate, inverted cones with average diameter and depth are positioned in a hexagonal arrangement (Fig. 5.20a). In Sec. 4.2.2, the area-weighted average diameter and depth are determined to be 1732 nm and 315 nm, respectively. In order to simplify the geometry of the optical model, the depth is rounded up to 320 nm. The back contact morphology of the optical model is obtained by the surface coverage algorithm (Sec. 4.2.3). The direction factor has been set to 0.75 to account for the directional formation of µc-Si:H films. Figure 5.20 depicts the morphology of the developed optical model.

The front contact morphology and the unit cell of the developed periodic substrate are shown in Fig. 5.20a. The surface textures represented by inverted cones in hexagonal arrangement are placed on top of a 500 nm thick flat ZnO:Al layer. Due to the hexagonal arrangement, the dimensions of the unit cell are different for \(x\)- and \(y\)-coordinate. For the cone diameter of 1732 nm, the period of the unit cell in \(x\)-direction is 1500 nm, while in \(y\)-direction is 2600 nm. The back contact morphology is shown in Fig. 5.20b. The total thickness of the µc-Si:H solar cell is assumed to be 1050 nm, where the thicknesses of p- and n-layer are 25 nm, while the thickness of the i-layer is 1000 nm. The back contact features are smoother, and the local film thickness is increased.

To compare periodic substrate (Fig. 5.20a) with the etched ZnO:Al substrate (Fig. 4.14a) and its quasi-random approximation (Fig. 4.14b), the surface coverage algorithm is used to determine the surface roughness and thickness gain for different i-layer thicknesses. The thicknesses of the p- and n-layer are kept constant and equal to 25 nm. The results are shown in Fig. 5.21.

Figure 5.21a depicts the surface roughness determined for an i-layer thickness up to 3 \(\mu\)m. Same as for the SnO\(_{2}\):F substrate (Fig. 5.15a), the surface roughness drops with increased i-layer thickness. Again, the change of surface roughness depends on the
Figure 5.21: (a) Surface roughness and (b) i-layer thickness gain of etched ZnO:Al substrate and its approximations as a function of the nominal i-layer thickness.

The surface roughness of the etched ZnO:Al substrate is 116 nm, while the quasi-random substrate exhibits roughness of 113 nm (Sec. 4.2.2). The surface roughness of the periodic substrate with a hexagonal arrangement of inverted cones can be estimated using the following relationship:

$$rms_{hex-cone} \approx \frac{D_{cone}}{\sqrt{21}}$$

where $D_{cone}$ is the depth of the cone structure. For the depth of 320 nm, the surface roughness is close to 70 nm. The surface roughness of the periodic approximation is smaller than for the etched ZnO:Al and quasi-random substrate. For a nominal i-layer thickness of 1 µm, the back contact roughness is 63 nm for the periodic substrate, which is a drop of 10%. For the etched ZnO:Al substrate, the surface roughness drops to 109 nm resulting in a decrease of 6%. For the quasi-random substrate, the drop of roughness is only 3%, and the back contact roughness is 110 nm. Compared to a-Si:H films deposited on textured SnO$_2$:F substrate (Fig. 5.15a), the change of the surface roughness is significantly smaller. This is influenced by the surface textures of the etched ZnO:Al substrate and directional film formation of µc-Si:H films. If the lateral dimensions of the surface textures are larger than the deposited film thickness, the back contact morphology exhibits only small changes. The same is valid for the directional film formation.

The i-layer thickness gain is shown in Fig. 5.21b. The thickness gain drops with increasing thickness of the i-layer. For a nominal thickness of the i-layer of 1 µm, the thickness gain for the etched ZnO:Al substrate is 4%. For the quasi-random and periodic substrate, the thickness gain is close to 3%. Consequently, the average thickness of the i-layer for the etched ZnO:Al substrate is 10 nm larger than for the quasi-random and periodic substrate. Since the morphology of the back contact does not exhibit significant changes, the thickness gain is small. Finally, the average thickness of the p-layer is also calculated. For the etched ZnO:Al substrate, the average p-layer thickness is 26.3 nm, while for the quasi-random and periodic substrate the average p-layer thickness is 25.8 nm.

Based on the results presented in Fig. 5.21, it can be concluded that the periodic substrate with a hexagonal arrangements of inverted cones can be used to model...
etched ZnO:Al and quasi-random substrate. Although the surface roughness of the front and back contact is smaller for the periodic substrate, the change of roughness is comparable for all substrates. Furthermore, the average thickness of the p- and i-layer is almost the same for all substrates.

As stated in Sec. 4.2.3, the surface coverage algorithm is not able to predict the formation of $\mu c$-Si:H natural textures. Consequently, the back contact morphology obtained by the surface coverage algorithm (Fig. 5.20b) is not a good description of the surface of $\mu c$-Si:H solar cells. To create an accurate description of the back contact of $\mu c$-Si:H solar cells, the natural textures have to be included in the model. To determine the size and shape of the natural textures, the surface of a $\mu c$-Si:H solar cell is measured using AFM. The fabrication and AFM measurements have been done at Malibu GmbH and Co. KG. In the first step, a 1000 nm thick $\mu c$-Si:H solar cell is deposited on an etched ZnO:Al substrate, and the film surface has been measured by the AFM. In the next step, an 80 nm thick ZnO:Al buffer layer is deposited on top of the $\mu c$-Si:H solar cell by a sputtering process. Finally, the surface of the ZnO:Al buffer layer is also measured by the AFM. The measured surfaces are shown in Fig. 5.22.

The measured surfaces of the deposited $\mu c$-Si:H solar cell and ZnO:Al buffer layer are shown in Figs. 5.22a and 5.22b, respectively. Due to the small thickness of the
5.3 Back contact losses in $\mu$-Si:H solar cells

ZnO:Al buffer layer, the natural textures of the $\mu$c-Si:H film are able to propagate through this layer. Consequently, the nanofeatures are present not only at the surface of the $\mu$c-Si:H solar cell (Fig. 5.22a), but also at the surface of the ZnO:Al buffer layer (Fig. 5.22b). In order to estimate the dimensions of the $\mu$c-Si:H natural textures, the large textures that originate from the front contact are filtered out [151].

The natural textures of $\mu$c-Si:H film are shown in Fig. 5.22c. The lateral dimension of the natural textures ranges from 100 nm to 200 nm. Due to the errors in the AFM measurement (Fig. 5.22c), the rms roughness of the natural textures cannot be precisely calculated. By removing areas with corrupted data, the rms roughness of the natural textures is estimated to be 10-12 nm. Figure 5.22d exhibits nanofeatures at the surface of the ZnO:Al buffer layer. The ZnO:Al buffer layer has little influence on the lateral size of the nanofeatures, which is almost the same as for the surface of the $\mu$c-Si:H solar cell. On the other hand, deposition of the ZnO:Al buffer layer makes the nanofeatures smoother. The rms roughness of the nanofeatures after the deposition of the ZnO:Al buffer layer is estimated to be 7-9 nm.

To create nanofeatures for the optical model, the image segmentation algorithm is used. In the first step, the individual $\mu$c-Si:H natural textures are identified. After the segmentation, the dimensions of individual features are determined. Assuming that the base of the individual features can be described by a square, it is determined that the average ratio between the height and period is 0.2. Finally, the individual features are replaced by a square base ellipsoids with the fixed height to period ratio of 0.2 (Fig. 5.23).

Figure 5.23a depicts the natural textures of the $\mu$c-Si:H solar cell, while the nanofeatures approximated by square base ellipsoids are shown in Fig. 5.23b. Relatively good agreement is observed between the natural textures and ellipsoid approximation. The rms roughness of the natural textures is 10 nm, while the quasi-random ellipsoids exhibit roughness of 11 nm. To complete the optical model, the ellipsoid textures are added on top of the back contact morphology (Fig. 5.24).

The morphology of the $\mu$c-Si:H solar cell with nanofeatures is shown in Fig. 5.24a. To create the morphology of the ZnO:Al buffer layer, it is assumed that the buffer layer has no influence on the big features that originate from the substrate. However, to account for the fact that the nanofeatures are smoother at the surface of the buffer layer, the rms roughness of the ellipsoid textures is reduced to 8 nm. Figure 5.24b
5. Influence of back contact on optical losses in silicon thin-film solar cells

(a) Morphology of μc-Si:H solar cell after adding artificial nanofeatures
(b) Morphology of ZnO:Al buffer layer with reduced roughness of nanofeatures

Figure 5.24: Surface morphology of a (a) μc-Si:H solar cell and (b) ZnO:Al buffer layer in the developed optical model.

depicts the morphology of the ZnO:Al buffer layer. The morphologies of the μc-Si:H solar cell and ZnO:Al buffer layer developed for the optical model (Fig. 5.24) nicely resemble the measured morphologies (Fig. 5.22).

5.3.3 Simulation results

To determine the back contact losses in μc-Si:H solar cells, the developed optical model is used to create simulation structures. The morphologies of the substrate, p-, i-, n- and ZnO:Al buffer layer are implemented into the FDTD solver with the corresponding optical properties. Again, the simulation settings from the flat simulations (Sec. 4.3.1) are used. The spatial step in x-direction is 15 nm, while in y-direction is 13 nm. Silver and aluminum are used as metal reflectors.

Silver reflector. To explain the experimental results (Fig. 5.19), the optical simulations are used to determine the back contact losses for the silver reflector with and without ZnO:Al buffer layer. Figure 5.25 depicts the cross sections of the simulated structures and corresponding power loss profiles. Since the unit cell is asymmetric, the cross sections and power loss maps can be shown for x- or y-direction. However, the power loss maps in x- and y-direction exhibit same trends. For the silver reflector, the cross sections and power loss profiles are shown for x-direction where the period is 1500 nm (Fig. 5.20). To show the interaction of light with the back contact, the power loss profiles are determined for a wavelength of 690 nm.

Figures 5.25a and 5.25b exhibit cross sections of the simulated solar cells with and without ZnO:Al buffer layer. Compared to the simulated a-Si:H solar cells (Figs. 5.16a and 5.16b), the change of the morphology is much smaller. Furthermore, the μc-Si:H natural textures are present at the back contact. The power loss maps are shown in Figs. 5.25c and 5.25d. The simulations show that the absorption in the silver reflector is high for the μc-Si/Ag back contact configuration (Fig. 5.25c). Consequently, less light is reflected back into the i-layer, where the absorption is reduced. For the solar cell with μc-Si/ZnO/Ag back contact (Fig. 5.25d), the absorption of the light in the silver reflector is lower, which results in an increased absorption in the i-layer.
5.3 Back contact losses in $\mu$-Si:H solar cells

To further investigate the back contact losses, it is necessary to determine the influence of the $\mu$-Si:H natural textures. Therefore, simulations are carried out for the back contact morphology without nanofeatures (Fig. 5.20b). The solar cells are simulated with and without ZnO:Al buffer layer. The results are shown in Fig. 5.26.

The cross sections of the simulated solar cells without nanofeatures are shown in Figs. 5.26a and 5.26b. Figures 5.26c and 5.26d exhibit power loss maps for a wavelength of 690 nm. By removing the nanofeatures, the absorption in the $\mu$-Si/Ag back contact (Fig. 5.26c) is significantly reduced, and the absorption in the i-layer is improved compared to the corresponding solar cell with nanofeatures (Fig. 5.25c). Similar trends are also observed for the solar cell with $\mu$-Si/ZnO/Ag back contact (Fig. 5.26d). When comparing the solar cells without nanofeatures, the influence of the ZnO:Al buffer layer is reduced. The absorption in the i-layer is almost the same with (Fig. 5.26d) and without (Fig. 5.26c) buffer layer. To make a detailed comparison of the simulated solar cells with the silver reflector, the quantum efficiency and absorption in the individual layers are determined.

Figure 5.25: Cross sections of simulated cells (a) without and (b) with ZnO:Al buffer layer. Power loss maps for (c) $\mu$-Si/Ag and (d) $\mu$-Si/ZnO/Ag back contact configuration (wavelength of 690 nm).
5. Influence of back contact on optical losses in silicon thin-film solar cells

Figure 5.26: Cross sections of simulated cells after removing nanofeatures (a) without and (b) with ZnO:Al buffer layer. Power loss maps for (c) μc-Si/Ag and (d) μc-Si/ZnO/Ag back contact configuration (wavelength of 690 nm).

Figure 5.27 depicts the absorption in the individual layers for μc-Si/Ag and μc-Si/ZnO/Ag back contact configurations with and without ZnO:Al buffer layer. For wavelengths shorter than 550 nm, the light does not reach the back contact and the absorption in the individual layers is the same for all simulated structures. For wavelengths longer than 550 nm, the absorption in the individual layers depends on the back contact morphology and configuration. Figures 5.27a and 5.27b exhibit absorption in the individual layers for solar cells with the nanofeatures. The back contact absorption is high for the solar cell without buffer layer (Fig. 5.27a). Consequently, the reflection losses and quantum efficiency are low. By introducing the ZnO:Al buffer layer, the back contact losses are reduced. This results in an increased quantum efficiency and larger reflection losses. The calculated short circuit density for the solar cell with μc-Si/Ag back contact is 16.8 mA/cm², while for the solar cell with μc-Si/ZnO/Ag back contact is 18.5 mA/cm². The difference of 1.7 mA/cm² is in a good agreement with the experimental results (Sec. 5.3.1).

The quantum efficiency and optical losses of solar cells without nanofeatures are
5.3 Back contact losses in $\mu$-Si:H solar cells

The simulated results show that the back contact losses of $\mu$-Si:H solar cells with the silver reflector are mainly influenced by the $\mu$-Si:H natural textures. The back contact losses can be reduced either by introducing a TCO buffer layer or removing the nanotextures at the interface with the silver reflector. As shown in Sec. 5.3.2, during the sputtering of a ZnO:Al buffer layer the roughness of the nanotextures is reduced. Therefore, the buffer layer reduces the back contact losses by improving reflectivity and making $\mu$-Si:H natural textures smoother.
5. Influence of back contact on optical losses in silicon thin-film solar cells

Figure 5.28: Cross sections of simulated cells (a) without and (b) with ZnO:Al buffer layer. Power loss maps for (c) \( \mu c\)-Si/Al and (d) \( \mu c\)-Si/ZnO/Al back contact configuration (wavelength of 690 nm).

**Aluminum reflector.** To further investigate the role of \( \mu c\)-Si:H natural textures, solar cells with aluminum reflector are simulated. In the first step, the solar cells with \( \mu c\)-Si:H natural textures are simulated with and without ZnO:Al buffer layer. From the simulations, the power loss maps are determined. The results are shown for \( y\)-direction with the period of 2600 nm (Fig. 5.28).

Figures 5.28a and 5.28b depict the cross sections of simulated solar cells with \( \mu c\)-Si/Al and \( \mu c\)-Si/ZnO/Al back contact configuration, respectively. Due to the \( \mu c\)-Si:H film formation, the back contact morphology is similar to the front contact and exhibits nanostructures. The influence of the ZnO:Al buffer layer on the absorption in the aluminum reflector can be observed in the power loss maps. Figure 5.28c depicts the power loss map without the buffer layer. The absorption in the aluminum reflector is much higher compared to the silver reflector (Fig. 5.25c). Due to the high absorption in the metal reflector, the light absorption in the i-layer is reduced. Figure 5.28d depicts the power loss map with the ZnO:Al buffer layer. The back contact absorption is now reduced and absorption in the i-layer is increased. Again,
5.3 Back contact losses in µc-Si:H solar cells

Figure 5.29: Cross sections of simulated cells after removing nanofeatures (a) without and (b) with ZnO:Al buffer layer. Power loss maps for (c) µc-Si/Al and (d) µc-Si/ZnO/Al back contact configuration (wavelength of 690 nm).

absorption in the aluminum reflector is higher than for the silver reflector (Fig. 5.25d).

In the next step, the influence of the µc-Si:H natural textures on the back contact losses in the aluminum reflector is investigated. The simulations are carried out for solar cells with smooth back contact morphology (Fig. 5.20b). The results shown in Fig. 5.29.

Figures 5.29a and 5.29b depict the cross sections of the simulated µc-Si:H solar cells with µc-Si/Al and µc-Si/ZnO/Al back contact configuration, respectively. The corresponding power loss profiles are shown in Figs. 5.29c and 5.29d. The back contact absorption in the solar cell with µc-Si/Al back contact configuration is high even with smooth back contact. This is influenced by the optical properties of aluminum. Compared to the µc-Si/Al back contact with nanofeatures (Fig. 5.28c), the absorption in the aluminum reflector is lower, and the absorption in the i-layer is increased. The power loss map for µc-Si/ZnO/Al back contact is shown in Fig. 5.29d. The buffer layer reduces the absorption in the aluminum reflector, and an increase of the absorption in the i-layer is observed.
5. Influence of back contact on optical losses in silicon thin-film solar cells

Figure 5.30: Calculated quantum efficiencies and optical losses for (a) µc-Si/Al and (b) µc-Si/ZnO/Al back contact with nanofeatures, and (c) µc-Si/Al and (d) µc-Si/ZnO/Al back contact without nanofeatures.

Figure 5.30 depicts a detailed comparison between the simulated µc-Si:H solar cells. The simulation results show that the quantum efficiency and absorption in the individual layers is different for wavelengths longer than 550 nm. In this wavelength range, the light reaches the back contact, and the performances of the solar cells are influenced by the back contact configuration and morphology.

Figures 5.30a and 5.30b exhibit the quantum efficiency and absorption in the individual layers of the simulated µc-Si:H solar cells where the nanofeatures are included. The solar cell with µc-Si/Al back contact exhibits high total absorption and back contact losses (Fig. 5.30a). Consequently, the reflection losses and quantum efficiency are low. The back contact losses are reduced for µc-Si/ZnO/Al back contact resulting in an improved quantum efficiency and increased reflection losses. From the simulated quantum efficiencies, the short circuit current densities are calculated. The solar cell with µc-Si/Al back contact exhibit short circuit current density of 15.1 mA/cm$^2$. The short circuit density of the solar cell with µc-Si/ZnO/Al back contact is 17.6 mA/cm$^2$.

Figure 5.30c exhibits the quantum efficiency and absorption in the individual layers of the solar cell with µc-Si/Al back contact without nanofeatures. The back contact losses are reduced compared to the corresponding solar cell with nanofeatures.
5.3 Back contact losses in $\mu$-Si:H solar cells

(5.30a). However, the change is not as large as for the silver reflector (Figs. 5.27a and 5.27c). Lower back contact losses improve the quantum efficiency and increase reflection losses. The quantum efficiency and optical losses of the solar cell with $\mu$-Si/ZnO/Al back contact with nanofeatures are shown in Fig. 5.30d. For aluminum reflector without nanofeatures, the influence of the buffer layer is larger than for the silver reflector (Fig. 5.27c and 5.27d), which is consistent with results for the a-Si:H solar cells (Fig. 5.17). The buffer layer further reduce the absorption in the aluminum reflector, and the quantum efficiency is increased. The short circuit current densities of the solar cells without nanofeatures are 16.1 mA/cm$^2$ and 17.8 mA/cm$^2$ for $\mu$-Si/Al and $\mu$-Si/ZnO/Al back contact, respectively.

Same as for the silver reflector, the $\mu$-Si:H natural textures have a large influence on the back contact absorption. The back contact losses are controlled by the ZnO:Al buffer layer, which improves the reflectivity of the back contact and reduces the roughness of the nanotextures at the interface with the metal reflector. To quantify the trade-off between the back contact absorption and the quantum efficiency, the simulated short circuit densities and optical losses of $\mu$-Si:H solar cell with silver and aluminum reflector are calculated.

Plasmonic and non-plasmonic back contact losses. The simulated results for $\mu$-Si:H solar cells with different back contact configurations and different back contact morphologies are summarized in Tab. 5.2. The simulations with a perfect absorber are used as a reference. The solar cell with $\mu$-Si/PA back contact exhibit highest back contact losses and lowest short circuit current density. Since all light that reaches the back contact is absorbed, the nanofeatures have no influence on the performance of the solar cell with $\mu$-Si/PA back contact. On the other hand, the simulation results show that the properties of the solar cells with $\mu$-Si/Al and $\mu$-Si/Ag back contact are significantly affected by the nanofeatures.

As shown in Sec. 5.1, the features with lateral size smaller than 200 nm are able to excite localized plasmonic resonances in silver and aluminum reflectors. For a silver reflector without the buffer layer, the plasmonic resonance enhances back contact absorption for wavelengths in the range 600 nm to 900 nm (Fig. 5.8a). Since in $\mu$-Si:H solar cells the light reaches the back contact for wavelengths longer than 550 nm (Fig. 5.27), the back contact losses for silver reflector are directly influenced by the plasmonic resonance. By removing the nanofeatures, the light cannot be coupled into the plasmonic resonance, and the back contact losses are reduced by 5.2 mA/cm$^2$ for $\mu$-Si/Ag back contact. For an aluminum reflector without buffer layer, the back contact absorption is enhanced for wavelengths in the range 400 nm to 500 nm due to the plasmonic resonance (Fig. 5.8b). The back contact absorption for the aluminum reflector is influenced by the tail of the plasmonic resonance since only wavelengths longer than 550 nm are able to reach the back contact (Fig. 5.30). Consequently, the back contact losses are reduced by 2.8 mA/cm$^2$ when nanofeatures are removed.

The optical approach to eliminate plasmonic absorption in the back contact is by introducing a TCO buffer layer. Since the perfect absorber does not exhibit plasmonic absorption, the back contact losses are reduced only by 2.5 mA/cm$^2$ after introducing a ZnO:Al buffer layer. Although the results from Sec. 5.1 show that back contact absorption in the perfect absorber can be increased when nanofeatures are present (Fig. 5.10a), this effect becomes negligible when complete solar cells are simulated. Consequently, for solar cells with $\mu$-Si/ZnO/PA back contact, there is no improve-
Table 5.2: Simulated short current densities and optical losses of \( \text{\( \mu \)} \text{c-Si:H} \) solar cells for different back contact configurations with and without nanofeatures.

<table>
<thead>
<tr>
<th>Back contact configuration</th>
<th>Short circuit current density with/(without) nanofeatures</th>
<th>Reflection</th>
<th>Back contact</th>
<th>Front contact</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mu \text{c-Si/PA} )</td>
<td>11.9/(11.9)</td>
<td>6.3/(6.3)</td>
<td>17.9/(17.9)</td>
<td>6.7/(6.7)</td>
</tr>
<tr>
<td>( \mu \text{c-Si/Al} )</td>
<td>15.1/(16.1)</td>
<td>8.3/(9.4)</td>
<td>11.6/(8.8)</td>
<td>7.8/(8.5)</td>
</tr>
<tr>
<td>( \mu \text{c-Si/Ag} )</td>
<td>16.8/(18.9)</td>
<td>9.8/(11.8)</td>
<td>7.7/(2.5)</td>
<td>8.5/(9.6)</td>
</tr>
<tr>
<td>( \mu \text{c-Si/ZnO/PA} )</td>
<td>13.2/(13.2)</td>
<td>7.1/(7.0)</td>
<td>15.4/(15.4)</td>
<td>7.1/(7.2)</td>
</tr>
<tr>
<td>( \mu \text{c-Si/ZnO/Al} )</td>
<td>17.6/(17.8)</td>
<td>10.0/(10.6)</td>
<td>6.4/(5.4)</td>
<td>8.8/(9.0)</td>
</tr>
<tr>
<td>( \mu \text{c-Si/ZnO/Ag} )</td>
<td>18.5/(19.1)</td>
<td>10.6/(11.4)</td>
<td>4.7/(3.0)</td>
<td>9.0/(9.3)</td>
</tr>
</tbody>
</table>

When the nanofeatures are removed. For the aluminum reflector, the ZnO:Al buffer layer reduces the back contact losses by 5.2 mA/cm\(^2\). The drop of back contact losses is larger than for the \( \mu \text{c-Si/Al} \) configuration after removing the nanofeatures. Therefore, the ZnO:Al buffer layer not only eliminates plasmonic losses, but also improves reflectivity of the back contact same as for the a-Si:H solar cells (Sec. 5.2.3). The plasmonic losses are removed since plasmonic resonance for the aluminum reflector is below 300 nm when ZnO:Al buffer layer is present (Fig. 5.8b). For the silver reflector, the back contact losses are reduced by 3 mA/cm\(^2\) after introducing the buffer layer. Unlike for the aluminum reflector, the back contact losses are reduced more by removing the nanofeatures then by introducing the buffer layer. Therefore, it can be concluded that \( \mu \text{c-Si/ZnO/Ag} \) back contact also exhibits plasmonic losses when the nanofeatures are present. As shown in Sec. 5.1, the ZnO:Al buffer layer shifts the peak of plasmonic resonance in the silver reflector to 450 nm (Fig. 5.8a). However, the tail of plasmonic resonance affects the absorption for wavelengths longer than 550 nm. After removing the nanofeatures, the back contact losses are further reduced by 1 mA/cm\(^2\) for \( \mu \text{c-Si/ZnO/Al} \) configuration and 1.7 mA/cm\(^2\) for \( \mu \text{c-Si/ZnO/Ag} \) configuration. The larger change for the silver reflector confirms that plasmonic losses are still present in that case. For the aluminum reflector, the back contact losses are reduced since smooth surface reflects better than nanotextured as shown for the perfect absorber (Fig. 5.10a).

The simulation results also show a trade-off between the back contact losses and the short circuit current. By reducing the back contact losses, the short circuit current density increases. Furthermore, the reflection and front contact losses are also increased. For silver and aluminum reflector, the short circuit current density can be increased by more than 2 mA/cm\(^2\) if the plasmonic losses are prevented.

### 5.4 Discussion and summary

In this chapter, the back contact losses of a-Si:H and \( \mu \text{c-Si:H} \) solar cells prepared on randomly textured substrates in superstrate configuration are investigated. In order to describe the experimentally realized solar cells, optical models are developed using periodic approximation. The front contact textures are described by geometrical structures, while a realistic formation of the silicon films is used to model the back
contact morphology. Furthermore, the nanotextures are taken into account when modeling the back contact morphology of $\mu$-Si:H solar cells. To quantify the back contact losses and gain understanding of the experimental results, the developed optical models are combined with FDTD simulations. From the simulated results, the influence of the TCO buffer layer and back contact morphology on the optical losses and the short circuit current is determined.

Experimental results and numerical simulations show that the back contact losses in a-Si:H solar cells prepared on randomly textured SnO$_2$:F substrates are reduced by introducing a ZnO:Al buffer layer. The drop of the back contact losses is calculated to be 1.1 mA/cm$^2$ for a silver reflector and 2.6 mA/cm$^2$ for an aluminum reflector. The experimental results show that the short circuit density is increased by 0.7/1.2 mA/cm$^2$ for the silver/aluminum reflector.

The numerical results show a good agreement with the experimental results. Based on the simulation results of metal reflectors (Sec. 5.1), it can be concluded that the investigated superstrate configuration a-Si:H solar cells do not exhibit plasmonic losses. Due to the smooth back contact morphology, the localized plasmonic resonances cannot be excited.

These conclusions are supported by separate experimental studies [67, 178]. In these studies, the ZnO:Al buffer layer has been nanotextured using wet etching approach or deposition of ZnO nanoparticles [67, 178]. Although the ZnO:Al buffer layer shifts the plasmonic resonance to 450 nm, the nanotextured silver reflector still exhibits the tail of plasmonic resonance, and the back contact losses are enhanced for wavelengths longer than 500 nm (Fig. 5.8a). On the other hand, a silver reflector without ZnO:Al buffer layer and with smooth morphology does not exhibit plasmonic losses. Consequently, the a-Si:H solar cells with a nanotextured ZnO:Al buffer layer exhibited lower short circuit currents compared to solar cells without a ZnO:Al buffer layer and with smooth back contact morphology [67, 178].

The developed optical model of $\mu$-Si:H solar cells and the simulated results exhibit a good agreement with experimental data from literature [123]. The back contact losses in the investigated $\mu$-Si:H solar cells are influenced by localized plasmonic resonances. Due to the columnar film formation, the back contact morphology is a superposition of the textures that originate from the front contact and $\mu$-Si:H natural textures. If the buffer layer is not present, the plasmonic resonance is directly excited for the silver reflector. For the aluminum reflector, the tail of plasmonic resonance influences the back contact losses. By depositing ZnO:Al buffer layer, the roughness of the nanotextures is reduced (Fig. 5.22), and the plasmonic resonances are shifted to shorter wavelengths (Figs. 5.8). Same as for a-Si:H solar cells [67, 178], the nanotextures excite the plasmonic absorption in the silver reflector due to the tail of plasmonic resonance. For the aluminum reflector, these nanotextures reduce the reflection properties of the back contact but they cannot excite the plasmonic absorption in the aluminum reflector with ZnO:Al buffer layer.

In order to achieve the best performance of $\mu$-Si:H solar cells, the morphology of ZnO:Al/metal reflector interface has to be smooth. This is confirmed by a recent experimental study where the ZnO buffer layer is deposited by LPCVD process [177]. LPCVD ZnO develops natural textures, which then enhance the plasmonic absorption in the silver reflector. The experimental study showed that by removing the nanotextures of LPCVD ZnO by an argon plasma treatment, the short circuit current density is increased by more than 2 mA/cm$^2$ [177].
5. Influence of back contact on optical losses in silicon thin-film solar cells

The ZnO:Al buffer layer plays an important role in reducing the back contact losses. The low refractive index of the ZnO:Al buffer layer influences the shift of plasmonic resonances to shorter wavelengths, and only the tail of plasmonic resonance can be excited. Furthermore, the sputtered ZnO:Al layer makes the nanotextures smoother and reduces the incoupling of light into the tail of plasmonic resonance. To completely remove the nanotextures, either thicker ZnO:Al layer should be sputtered or an argon plasma treatment should be used.

The highest short circuit currents can be achieved by using silver reflectors. However, if the back contact exhibits nanofeatures, plasmonic losses will occur, and performances are reduced. On the other hand, aluminum reflectors do not exhibit plasmonic losses, but their optical properties are poor. Consequently, the short circuit currents of silicon solar cells with aluminum reflectors are smaller. As an alternative, white paint reflectors can also be used [31, 33, 177]. The white paint does not exhibit plasmonic losses, and it behaves like a quasi-Lambertian scatterer [113]. The fabrication costs of back contacts with aluminum or white paint reflectors are smaller than for silver reflectors. However, the white paint reflectors require a thick TCO buffer layer [31, 33, 177], which increases the fabrication time of solar cells. To determine the optimal back contact configuration for silicon thin-film solar cells, all these considerations have to be taken into account.
Part IV

Outlook
Chapter 6

Conclusions and future investigations

In this study, optoelectronic devices with nanostructured layers and nanostructured interfaces were investigated. The investigation was conducted by experimental measurements and optical modeling. Modeling of optoelectronic devices is crucial for explaining experimentally measured data and gaining insights into operating principles. Furthermore, modeling helps to identify problems and improve performances of optoelectronic devices.

The first step in creating an accurate model of an optoelectronic device is to properly describe its geometry. This includes not only the thickness of the device layers, but also the morphology of its interfaces. In the next step, materials that are used to fabricate the device are represented by optical constants, which are then included in the model. Finally, to model the performance of the optoelectronic devices, it is necessary to determine the light propagation within the device. This is achieved by solving Maxwell’s equations for the developed model.

The most accurate approach to solve Maxwell’s equations is to use analytical methods. However, these approaches are only accurate for optoelectronic devices with flat interfaces and nanostructured layers. In this study, the analytical methods were used to model the transparent photodetector, standing wave and Fabry-Perot spectrometer. For the complex geometries that are present in optoelectronic devices with nanostructured interfaces, Maxwell’s equations are solved numerically. Therefore, to investigate silicon thin-film solar cells deposited on randomly textured substrates, a FDTD solver was used.

To confirm the accuracy of the developed models, the performances of the optoelectronic devices that are calculated using analytical or numerical methods are typically compared to experimentally measured data. In the first part of this study, the calculated transmission and quantum efficiencies of the transparent detector showed excellent agreement with measured data (Fig. 2.14). A good agreement between experimental and calculated data was also observed for the models of the standing wave spectrometer (Figs. 3.18 and 3.19) and Fabry-Perot spectrometer (Figs. 3.26 and 3.27).

In the second part of the thesis, experimentally fabricated silicon thin-film solar cells with and without ZnO:Al buffer layer were simulated using the FDTD solver and developed optical models (Figs. 5.14, 5.20 and 5.24). Again, the simulated data (Fig. 5.17 and 5.27) showed good agreement with experimentally measured data (Figs. 5.13 and 5.19). Finally, the developed models were used to explain the behavior
Figure 6.1: Sagnac setup for standing wave spectrometer based on a transparent photodetector [187].

of experimentally realized optoelectronic devices.

From the optical models, the limitations of the device can be determined. Consequently, new strategies can be developed to improve the performances of the device. In some cases, it is necessary to improve the optical model itself to correspond better to experimental results. In the following sections, different approaches on how to improve the performances of the standing wave spectrometer and optical models for silicon thin-film solar cells are presented.

6.1 Spectral imaging with transparent photodetector

The linear setup of the standing wave and Fabry-Perot spectrometer allows for the realization of 2D spectrometer arrays, which is very promising for spectral imaging. However, this study has shown that the lower operating range of these devices is limited by the Fabry-Perot resonator and widening of the spectral lines (Eq. 3.40). The Fabry-Perot resonator is formed between linearly arranged elements of the standing wave and Fabry-Perot spectrometer. To create a spectrometer based on the transparent photodetector with increased operating range, the linear setup has to be avoided. The standing wave spectrometer in a non-linear setup can be achieved by using Sagnac geometry [186, 187].

Figure 6.1 exhibits standing wave spectrometer based on the transparent photodetector in Sagnac setup. In this configuration, the input beam is divided by the beam splitter. The refracted beam travels along one arm, while the transmitted beam travels along the second arm of the spectrometer. The refracted and transmitted beam are then recombined. Since the beams travel in opposite directions, a standing wave is formed. To record the standing wave pattern it is necessary to move the transparent photodetector. For different positions of the transparent photodetector, different part of the standing wave is located within the absorber layer and output signal is
6.1 Spectral imaging with transparent photodetector

modulated by the standing wave pattern.

In Sagnac configuration, the formation of a Fabry-Perot resonator is prevented. Consequently, the output signal is described only by a cosine function \([187]\). The appearance of higher order harmonics is eliminated from the spectrum that is obtained by a Fourier transform. The operating range of the standing wave spectrometer in Sagnac configuration is determined by the visibility of the spectrometer.

The presented setup of the standing wave spectrometer (Fig. 6.1) can be used for the realization of a single pixel for a spectral imaging camera. To create 2D spectrometer arrays, dense integration of transparent photodetectors on a single chip is needed. However, this configuration does not allow that.

Figure 6.2 depicts the standing wave spectrometer in Sagnac configuration with multiple transparent photodetectors on a single chip. Due to the configuration, an intermixing of spatial and spectral information occurs. As shown in Fig. 6.2, the light from one spatial position interferes with the light from different position. Consequently, the spatial image and spectral information are not properly recorded. The presented configuration also exhibits problems if the coherence length of a light source is small. In order to sample the standing wave, the transparent photodetector has to be placed at the position where the path difference between the refracted and transmitted light is zero, which cannot be realized in the presented configuration. To overcome this problem, Sagnac configuration with optical fibers can be used \([186, 187]\). However, the intermixing of the spectral and spatial information for densely integrated transparent photodetectors remains an issue even for this realization.

To solve the problem with intermixing of the spatial and spectral information, the Sagnac configuration has to be modified. This can be simply achieved by removing one mirror and realizing a Sagnac spectrometer in a triangular configuration. Again, the transparent photodetector has to be moved in order to record the standing wave. As an alternative, configuration with stationary transparent photodetector that also prevents intermixing can be realized as shown in Fig. 6.3. To achieve this goal, a penta prism has to be included instead of one mirror. The penta prism inverts...
Figure 6.3: Standing wave spectrometer in modified Sagnac configuration without intermixing of the spatial and spectral information.

the spatial positions and eliminates intermixing. To place the chip with transparent photodetectors at the position where the path difference between the refracted and transmitted light is zero, a porro prism can be used. The porro prism allows for the realization of spectrometer with equal arms length. Furthermore, in this configuration the standing wave is sampled by moving the porro prism. Using this approach, the chip with the transparent photodetectors is stationary, which is good for the electric connectors.

High accuracy spectral imaging cameras based on the standing wave spectrometer can be achieved by using the modified Sagnac configuration. However, the geometry of the setup is no longer linear. Alternative approach to realize high accuracy spectral imaging camera, is to use the Michelson spectrometer setup, where a chip with detector arrays is used to record spectral information. The spectrometers with a linear setup can be used for the development of cheap spectral cameras where a high accuracy or increased operating range is not needed. The next step in the spectrometer research is to realize a standing wave spectrometer in a modified Sagnac configuration and determine its performances.

6.2 Improved optical modeling of thin-film solar cells

The investigation of back contact losses in silicon thin-film solar cells (Chpt. 5) was based on the assumption that periodic substrates can be used to approximate random (Figs. 4.8 and 4.12) or quasi-random substrates (Figs. 4.10b and 4.14b). The dimensions of the periodic substrates were equal to area-weighted average features (Figs. 5.14a and 5.20a), which were determined by the image segmentation algorithm (Sec. 4.2.2). By comparing different substrates, it has been shown that they exhibit similar change of surface roughness and increase of the i-layer thickness. However, the rms roughness of the periodic substrates was lower (Figs. 5.15a and 5.21a).
6.2 Improved optical modeling of thin-film solar cells

Figure 6.4: Influence of nominal i-layer thickness on (a) surface roughness and (b) i-layer thickness gain of textured SnO\textsubscript{2}:F substrate and its approximations.

developed optical models were able to explain the experimental results and provide deeper understanding of the back contact losses, but the simulated quantum efficiency and total absorption were different compared to the experimental results. To predict the performance of the experimentally realized solar cells and accurately investigate the light trapping properties of different substrate morphologies, the optical model has to exhibit better agreement with experimental results.

In Sec. 5.2, the investigation of a-Si:H solar cells prepared on a randomly textured SnO\textsubscript{2}:F substrate (Sec. 5.2.2) has been conducted by area-weighted average feature to generate a periodic substrate. For this substrate (Fig. 5.14a), the period of pyramidal textures is 400 nm, the height is 110 nm, and the rms roughness is 25.9 nm (Eq. (5.3)). On the other hand, the randomly textured SnO\textsubscript{2}:F substrate exhibits roughness of 36.9 nm, while the rms roughness of the quasi-random substrate is 40.3 nm. To improve the optical model, the rms roughness of the periodic substrate has to match the roughness of the random or quasi-random substrate. By using quasi-random substrate as a reference, the height of the pyramid for the periodic substrate has to be 170 nm, which is determined from Eq. (5.3). The period of the pyramid texture is then 630 nm, which is calculated from the average height to period ratio of 0.27 (Sec. 4.2.2). To compare this periodic substrate with random and quasi-random substrate, the surface coverage algorithm for a-Si:H films is used to determine the surface roughness and average i-layer thickness. The nominal thickness of the i-layer is varied, while the thickness of the p- and n-layer is fixed to 10 nm. The results are presented in Fig. 6.4 for all investigated substrates.

The change of the surface roughness with an increase of the nominal i-layer thickness is shown in Fig. 6.4a. The periodic substrate with matched rms roughness exhibits excellent agreement with the quasi-random substrate. Furthermore, the agreement with the random substrate is better than for the periodic substrate based on the average feature. Figure 6.4b exhibits the thickness gain of the i-layer. It can be observed, that the thickness gain of the periodic substrate with matched roughness exhibits better agreement with the random substrate. For a 320 nm thick a-Si:H solar cell, the back contact roughness for the periodic substrate with matched roughness is 36.7 nm. This value is almost equal to the quasi-random substrate (Sec. 5.2.2). The i-layer thickness gain is 11.6 %, which is slightly smaller than for the random
6. Conclusions and future investigations

Figure 6.5: Calculated quantum efficiencies and optical losses for a (a) random substrate, (b) quasi-random substrate, (c) periodic substrate with match rms roughness and (d) periodic substrate based on average feature size.

The accuracy of the periodic substrate with increased roughness, FDTD simulations are used. In the first step, the random (Fig. 4.10a) and quasi-random substrate (Fig. 4.10b) are simulated, and these results are used as a reference. To create the interface morphologies for the simulations, the surface coverage algorithm is used. The thicknesses of the p-, i- and n-layer are assumed to be 10 nm, 300 nm and 10 nm, respectively. To improve the agreement with experimentally realized solar cells, it is taken into account that the optical properties of the silver film deposited on the rough surface are not equal to those of the bulk silver (Sec. 5.2.3), and optical properties of porous silver are used [182, 183].

For the random and quasi-random substrate, the simulation area is 2.5 x 2.5 µm². After the simulation of random and quasi-random substrate, the periodic substrates have been simulated. For the periodic substrate based on the area-weighted average feature, the period and height of the pyramid texture are again 400 nm and 110 nm, respectively. On the other hand, for the periodic substrate with matched roughness, the period is 630 nm and the height is 170 nm. From the simulated electric field distributions, absorption in the individual layers of the simulated solar cells has been
Table 6.1: Simulated short circuit current densities and optical losses of a-Si:H solar cells for different optical models.

<table>
<thead>
<tr>
<th>Optical model</th>
<th>Simulated optical absorption (mA/cm²)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Short circuit current density</td>
</tr>
<tr>
<td>random substrate</td>
<td>15.1</td>
</tr>
<tr>
<td>quasi-random substrate</td>
<td>15.0</td>
</tr>
<tr>
<td>periodic substrate (roughness)</td>
<td>14.9</td>
</tr>
<tr>
<td>periodic substrate (average feature)</td>
<td>14.7</td>
</tr>
</tbody>
</table>

calculated. The results are shown in Fig. 6.5.

The absorptions in the individual layers for the random (Fig. 6.5a) and quasi-random substrate (Fig. 6.5b) are almost equal, which confirms that the quasi-random substrate is a good approximation of the random substrate. Figure 6.5c exhibits the quantum efficiency and optical losses for the periodic substrate with matched roughness. The agreement with reference results is good. The back contact absorption is slightly smaller for wavelengths longer than 750 nm, but the overall trends are the same. On the other hand, the periodic substrate based on the average feature (Fig. 6.5d) exhibits less agreement with the reference results. For this optical model, the back contact losses display absorption peaks, which are not present in other cases. Both periodic approximations exhibit higher reflectivity for shorter wavelengths compared to the reference results, which is again influenced by the fact that a single texture is not able to match the light incoupling of random substrates (Sec. 5.2.3). To quantify the agreement between different optical models, optical absorptions in the individual layers are converted into current densities. The results are presented in Tab. 6.1.

The simulation results show that the short circuit current densities and optical losses of the random and quasi-random substrate are almost the same, which confirms excellent agreement between these two substrates. The simulated short circuit current density is also in a good agreement with the experimental results (Sec. 5.2.1). The periodic substrate with matched roughness exhibits similar short circuit current density. Compared to random and quasi-random substrate, the reflection losses are increased, while the front and back contact losses are slightly reduced. The short circuit current density for the periodic substrate based on the average feature is the smallest, while the reflection and back contact losses are the highest.

Based on the presented results, it can be concluded that the best optical modeling of the fabricated a-Si:H solar cells is achieved by using random substrate. However, these simulations are time consuming. The simulation time of the periodic substrates is 10 times shorter than for the random or quasi-random substrate. For the periodic approximations, better agreement is achieved if the periodic substrate exhibits matched roughness. To confirm these conclusions, it is necessary to repeat the investigation for the etched ZnO:Al substrate with deposited µc-Si:H solar cells.
Finding the best periodic approximation of a randomly textured substrate is also important for light trapping investigation. Recent experimental investigations have been unable to determine if periodic or random substrates are better for light trapping in silicon thin-film solar cells [33]. Furthermore, for the periodic substrates it is determined that the best light trapping properties are achieved if the period of the surface textures is comparable to the film thickness [68]. Therefore, the light trapping properties of the periodic substrates are reduced if the film thickness does not correspond to the period of the substrates. On the other hand, randomly textured substrates do not exhibit this problem. By using a periodic approximation based on the matched roughness, randomly textured substrates can be further investigated, which can lead to development of substrates with optimal light trapping properties.
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List of publications related to this research


Other publications


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