Investigation and Simulation of the Optical Properties of Doped Silicon

University of Constance
Faculty of Physics
Chair of Prof. Dr. E. Bucher

Presented by
Wolfgang Stumpf

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Abstract

This work summarizes studies in a project work of the optical properties of electrical grade polycrystalline doped silicon (Si) wafers for industrial solar cells. The focus was set on varying high doping rates of phosphorus for the reverse side contact and aluminium as a back surface reflector of the solar cell. The work also included the calculation of the degree of ionization at room temperature using the numerically solved neutrality condition involving the Fermi integrals. The optimization of the light confining geometry in the near infrared wavelength range was done by use of a ray tracing simulation program and analytical calculation of the solutions for reflectance $R$ and transmittance $T$ concerning single-, double- and $n$-layer antirefection coatings. For the latter the matrix method has been used. The optical loss from excessive doping at the backside for a back surface field has been quantified and studied. It has been shown that the doping is not a limit for charge carrier generation below and in the range of the band edge.
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Introduction

Several approaches to increase solar cell efficiency exist. Wavelengths of an energy below the band gap of the semiconducting material solar cells consist of can pass the cell without significant absorption. An idea is to confine the light by trapping into the solar cell, thereby increasing the optical path length by to and fro reflections inside the cell. The optical path elongated in that way increases the probability of absorption and free charge carrier generation. Excessive doping at the backside is favorable for two reasons: On the one hand, the dopant excess forms an electric field so-called back surface field (BSF) that enhances free charge carrier separation and the electrical contact. On the other hand it can act as a back surface reflector (BSR). This rises need to optimize back surface reflectance with respect to parasitic absorption.

Computer simulations supplied the studies of various cell front and back texturizings with different reflectance behavior and anti-reflection coatings (ARC). To fit simulation parameters to real conditions and to include the changes in spectral absorption behavior, measurements of silicon wafers of high and low doping rates with different dopants have been performed in the infrared (IR) region below the band gap energy of silicon. An extensive literature research that preceded the work did not reveal any solutions to the specific problem.

Several experiments of the advanced practical course of the University of Constance formed the basis for the project work: “Solar Cells”, “Tunnel Effect in Silicon”, “Hall Effect in Semiconductors” and “Surface Plasmons”. In addition a seminar talk on semiconductor devices and alternative energies was given during the summer term 2001 titled “Organic Solar Cells and Lasers” and furthermore the elective course “Semiconductor Physics and its Application” has been attended and deepened during the exercise course. At this stage, the final exam of elective course “Alternative Energies” was successfully passed.
Measurement techniques

First of all the used measurement techniques will be mentioned and their principles explained.

2.1 The spectral photometer Cary 5

The device available at the chair of Prof. Dr. Bucher built by the company Varian (Australia) is a powerful optical tool for transmission measurements. It has been originally developed for chemical analysis of cuvettes in the ultraviolet (UV), visible (VIS) and near infrared (NIR) spectral range. It is also useful for measurements on semiconductors and metals. The device is also capable of reflectance measurements. For that purpose, an Ulbricht sphere has been installed as an additional part. Details concerning the theory of the Ulbricht sphere will be treated detailed in section 2.4.

2.2 Experimental setup

The experimental setup, i.e. the interior assembly of the Cary 5, is schematically illustrated in figure 2.1.

![Figure 2.1: Interior assembly of the spectral photometer Cary 5. Modified from [1].](image-url)
The light source is a tungsten–halogen bulb lamp for the VIS and the NIR. In the ultraviolet a deuterium lamp replaces it. The lamps are mounted on a cylinder that can be rotated by its roll axis for alternating operation in the required spectral range. The mirror N1 works as concentrator of the light from the well, that is reflected by the mirror arrangement from N2 to N4 and collected in slit S1. S1 is a turnable wheel with six different positions. Five of these embody an appropriate filter to assist the monochromatizing. Thus, the light passes one of the five filters which wavelength range is given in table 2.1.

<table>
<thead>
<tr>
<th>Wavelength in nm</th>
<th>Filter</th>
</tr>
</thead>
<tbody>
<tr>
<td>175 – 340</td>
<td>No Filter</td>
</tr>
<tr>
<td>340 – 570</td>
<td>White Filter (WG 320)</td>
</tr>
<tr>
<td>570 – 800</td>
<td>Orange Filter (OG 530)</td>
</tr>
<tr>
<td>800 – 1200</td>
<td>Red Filter (RG 780)</td>
</tr>
<tr>
<td>1200 – 2000</td>
<td>Silicon Interference Filter</td>
</tr>
<tr>
<td>2000 – 3300</td>
<td>Germanium Interference Filter</td>
</tr>
</tbody>
</table>

Table 2.1: Transmittance range of the different filters [1].

The width of the slits S1 – S3 are mechanically coupled to each other and can be varied in size of their aperture according to the desired resolution by a microprocessor driven stepping motor. This will be explained later in detail. The light gets at last to the monochromator. It is reflected at the large collimation mirror N5a under an angle of 8° (upwards, not displayed in the scheme) and arrives to the rotatable diffraction grating G1 where it is split by dispersion in its consisting wavelengths. Its position decides which wavelength will be imaged on the subsequent slit. The monochromatic constituents are anew reflected at N5a and at mirror N6. The central slit S2 confines them afterwards. From here, the light arrives at the second monochromator (with collimation mirror N5b and diffraction grating G2), which is laterally reversed built up to the first and working identical. It filters out eventually occurring aberrations due to the first by its special geometry. The parameters of the grating G1 are compiled in table 2.2.

<table>
<thead>
<tr>
<th>Grazing parameter</th>
<th>NIR</th>
<th>UV–VIS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimensions</td>
<td>70 x 45 mm</td>
<td>70 x 45 mm</td>
</tr>
<tr>
<td>Blaze angle</td>
<td>10.3°</td>
<td>8.5°</td>
</tr>
<tr>
<td>Reciprocal Dispersion</td>
<td>0.98 nm/mm</td>
<td>3.92 nm/mm</td>
</tr>
<tr>
<td>Lines per mm</td>
<td>1200</td>
<td>300</td>
</tr>
</tbody>
</table>

Table 2.2: Parameters of the diffraction gratings [1].

The diffraction gratings G1 and G2 are double-sided. Their front and reverse sides are especial coordinated (“front–to–back–accuracy”) blazed gratings. One side is appointed to the diffraction in the NIR, the other to the diffraction in the UV–VIS. At 800 nm the gratings are be rotated by 180° according to this. In the recorded spectra this can be easily seen by a characteristically kink in the measured curve. The distance between the grating lines of the NIR is four times larger than for the UV–VIS grating and hints that the spectral bandwidth (SBW) of the NIR grating is curtly four times bigger than the SBW of the UV–VIS grating. This becomes particularly clear for the value of the reciprocal dispersion because it quantitatively denotes the amount of spectral range per length unit that will be diffracted into position space. Effectively from the wavelength continuum approximately

\[ \text{This discontinuity is at 820 nm and has additional the following reasons: Not only the gratings are rotated by 180°, but also the preferred direction of the polarization by 90° with them because the gratings and furthermore the detectors are changed. This becomes especially clear for a transmission measurement of a polarizing slide. For example, this has to be taken into account for solar cells, which are provided with a texture pattern.} \]
only the SBW +/- 2 nm remains after the second monochromator. Thus the stray light is reduced. The size of S3 determines in combination with the size of S1 the SBR of the device. A narrow slit means a small SBW. Which wavelength arrives in the end at the sample, is determined by the SBW and the grating position. For example if a SBW of 2 nm is chosen and the selected wavelength is 678.5 nm the range from 676.5 nm to 680.5 nm comes to the sample. The light leaving the second monochromator is reflected at the mirror N7 into the chopper N8, which is an essential part of the device. The chopper also allows the alternating usage of the light for measurement and reference. It consists of a slab with two areas, which is rotated under an angle of 45° to the light beam. One part is mirrored–glass and reflects the beam in turn on N9S respectively N9R to the sample area. The counterpart is dull blackened, by which the arriving signal at the detector can be corrected to the dark current. In the sample area the light is split into measurement and reference beam. The sample to be measured is placed into the beam path of the measurement beam and the reference beam remains unaffected for absolute measurements. For reference measurements a reference sample can be mounted. And if the measured sample absorbs too much for example a grey filter.

After the sample chamber (dashed plotted in figure 2.1) both partial beams are brought together by N10S and N10R plus the additional mirrors from N11 to N13 for each at the corresponding detector. There are two detectors available: A photomultiplier tube (PMT) for the UV–VIS and PbS semiconductor detector for the NIR. Not in the drawing is the mirror Z which one is positioned that way to shield the thermal radiation coming from the chopper motor against the sensitive semiconductor detector for the NIR. By turning the mirrors N10R and N10S away, between both detectors can be switched. The rotational motion of the gratings around their center allows recording a continuous spectrum because the wavelength at the slit S3 is determined by each of their position. The rotational motion only takes place during the phases of the chopper cycle when no measurement is performed. For 30 measurement cycles per second this means that one needs a stepper motor which is able to perform high acceleration / brake applications without vibrations or backstrokes. The microprocessor driven stepper motor in the Cary 5 complies with the technical requirements and rotates the grating with a velocity of 16000 nm/min for the UV–VIS as well as 64000 nm/min for the NIR. The adjustable time for the measurement sets the amount of chopper cycles for a measurement at a certain wavelength. The measured values at a fixed wavelength will be averaged afterwards (signal averaging time). The step width of the wavelength difference between the measurement points is adjustable from 1 to 4 micron for the Cary 5.
2.3 Lambertian behavior

This section gives a short explanation about diffuse and directional reflectance (and transmittance) of light. Light that undergoes reflection or is transmitted, consists of two fractions: a directional and a diffuse. In this terms diffuse means without a preferred direction and directional means the intensity depends on the direction. This directional dependence is also called lambertian. It is defined by (Lambert’s law) [2]:

\[ J(\vartheta) = J_0 \cos(\vartheta) \]  

(2.1)

In top view, a surface area element that is rotated by the angle \( \vartheta \) with respect to the surface normal appears shrunked by the cosine factor in equation (2.1). The same holds true for the radiation intensity \( J \) (units: \( \text{W sterad}^{-1} \)), what is origin for the characteristics of a non–lambertian surface area (see figure 2.3) that usually is extended in normal direction. A Lambert factor of nought denotes total directional dependent characteristics; a Lambert factor of one stands for complete diffuse characteristics.

![Figure 2.2: Radiation intensity for a surface corresponding to Lambert’s law.](image)

2.4 The Ulbricht sphere

The Ulbricht sphere is also called integrating sphere because it averages over influences by incidence angle, shadow forming, modes, polarization and inhomogeneities e.g. in the beam profile. That way errors in the measurement, which usually occur by the influence of these parameters, are avoided. The integrating sphere is quite suitable for diffuse reflectivity measurements.

Sumpner and Ulbricht already pointed out the principle of the Ulbricht sphere 100 years ago. In short words it is a hollow sphere, whose inner surface is highly reflecting over a wide spectral range [3]. This reflectance is not directional (diffuse). That means the light is rejected in many different directions for example due to a strong surface roughness. Light that arrives at the inner surface of a hollow sphere that is internally coated with a highly reflecting material is multiple times reflected until it is uniformly distributed in the sphere.

The radiant flux that comes in the end to the detector is proportional to the total radiant flux in the sphere. By that spatial collection principle of light it is possible to determine the total emission of a light source (lamp, laser, LED, etc.). Fabrication and design of such an optimized integrating sphere is still a non–trivial problem and is based upon experience. For the design there are two important parameters: throughput \( \tau \) and stability. The throughput\(^2\) is defined as the ratio of the radiant flux at the exit of the sphere (e.g. at the detector) to the radiant flux at the entrance [3]:

\[ \tau = \frac{\Phi_i}{\Phi_o} = \frac{\rho A f_o}{(1 - \rho) \cdot (1 - A f_o)} \]  

(2.2)

\(^2\)The formulas for the Ulbricht sphere will be discussed in section 2.5 more in detail.
§2.4 The Ulbricht sphere

The variables in equation (2.2) are:

- $\tau$ = Throughput
- $\Phi_i$ = Input radiant flux in [Watt]
- $\Phi_o$ = Output radiant flux in [Watt]
- $\rho$ = Reflectivity of the wall of the sphere in %
- $A$ = Ratio of the aperture areas
- $f_o$ = Ratio of the output area to the total surface area of the sphere
- $f_a$ = Ratio of all aperture areas to the total surface area of the sphere

In easy words this means that for constant ratios of the aperture areas smaller spheres have a larger throughput than bigger ones. This can be easily seen from the inverse proportionality to the surface area — it would become especially significant for small reflectivity of the coating. For the stability of the Ulbricht sphere the ratio of the total surface of all apertures and inner troubles to the total inner surface must be clearly smaller than 5% [3]. By that it is necessary to find a middle way between small diameter for optimizing the throughput and a large diameter for enhancement of the stability. The total inner surface area should be as large as possible compared to the aperture areas. And the sphere should have a highly diffuse reflecting (the directional fraction minimized), constant in the spectrum and fluorescent free as an ideal inner coating material. The Ulbricht sphere is an essential part of the Cary 5. The sphere used in this device has a diameter of 110 mm and is internally coated with the material BaSO$_4$. There are also other coatings that show better specific properties, for example Optisol, based on polytetrafluoroethylene (PTFE).

![Figure 2.3: Beam path for diffuse reflectivity measurements [1].](image)

Figure 2.3 schematically illustrates the beam path ending up into the sphere in the device for both of measurement and reference beam. The measurement beam (sample beam in figure 2.3) is reflected by the concave mirror M1 and the mirror M2 on a lens, which focuses the beam to a sample that is slightly bevelled mounted at an aperture of the sphere. The angle is about 3°20′ to the normal of the sample beam and therefore integrates a directional fraction of the reflection into the measurement, which would under an angle of 0° to the normal exit the sphere again through the aperture of the sample beam. This is exploited for determination of the diffuse reflectance part of a single sample.

The reference beam is diffusely in-coupled at another aperture of the sphere. The ratio of the aperture area to the total inner surface area of the Ulbricht sphere that has been used is about 3%. The character of the measurement is always a comparison between measurements. That means for assigning the absolute reflectivity of an unknown sample to a reflectance spectrum of a reference sample with an exactly defined reflectivity. The reflectance spectrum of the reference sample will be designated as baseline and had to be recorded before the actual measurements. The baseline for a certain measurement required a reference sample whose reflectivity had to be chosen as close as possible to the reflectivity of the sample.
Transmittance measurements can be done in addition by help of the Ulbricht sphere just by mounting a reflector in the place of the sample. The sample itself is put in the beam path on the opposite side over the sample beam aperture.

![Figure 2.4](image_url)

**Figure 2.4:** (a) Application of the Ulbricht sphere for reflectance measurements and (b) for transmission measurements depicted here for the sake of simplicity as a single beam setup (Taken from [3]).

### 2.5 Formulas of the Ulbricht sphere

The averaged illumination power $\overline{E}$ in units of [Jm$^{-2}$] at the inner part of the sphere can be composed of a direct and an indirect fraction (see section 2.3 and [4]):

$$\overline{E} = E_{\text{ind}} + E_{\text{dir}}$$  \hspace{1cm} (2.3)

The irradiated power $\Phi_L$ will be completely absorbed:

$$\Phi_L = \Phi_a = \overline{E} \cdot A_K \cdot \alpha = \overline{E} \cdot A_K \cdot (1 - \rho)$$  \hspace{1cm} (2.4)

The indirect illumination power $E_{\text{ind}}$ is constant over the total inner surface area $A_K$. It can be calculated from:

$$E_{\text{ind}} = \overline{E} - E_{\text{dir}} = \frac{\Phi_L}{A_K \cdot (1 - \rho)} - \frac{\Phi_L}{A_K}, \text{ with } E_{\text{dir}} = \frac{\Phi_L}{A_K}$$

$$E_{\text{ind}} = \Phi_L \cdot \frac{\rho}{A_K \cdot (1 - \rho)} = \Phi_L \cdot C_K$$  \hspace{1cm} (2.5)

In equation (2.5), $C_K$ is a constant of the sphere. The measurement of the indirect illumination power at an arbitrary place in the sphere is a ratio for the total light flux generated in the sphere

$$E_{\text{ind}} = \frac{\Phi_L}{C_K}.$$  \hspace{1cm} (2.6)

That explains the composition of the formula for the throughput $\tau$ (2.2). It is easy to see that:

$$A_K \triangleq 1 - Af_a$$  \hspace{1cm} (2.7)

whereby for better survey the right side is normalized to dimension equal unity.
2.6 Four–point measurement of the electrical resistance

The four–point measurement of the electrical resistance is required to appoint the conductivity of the doped silicon wafer. From the conductivity conclusions can be drawn to give a clue for the available charge carrier density $N$.

$$ R = \frac{l}{e_0 N \mu A} \quad (2.8) $$

$R$ is the measured resistivity, $e_0$ the elementary unit charge and $\mu$ the mobility of the corresponding charge carriers. $A$ denotes the cross section of the sample and $l$ its length. If the ohmic resistance of the cables and contacts is of the same order as the electrical resistance of the sample in measurement, the usual two–point method is burdened by a to large error. The four–point method is an elegant enhancement of the two–point method what is insightful from the calculation. It can easily be seen in the following figure 2.5, that:

$$ U = (I - IV_1) \cdot R_{\text{sample}} $$
$$ U = (R_1 + R_2 + R_{\text{internal}}) \cdot IV_1 $$
$$ U_1 = R_{\text{internal}} \cdot IV_1 \quad (2.9) $$

$U$ is the voltage drop at the ohmic resistance of the sample; $U_1$ the voltage measured by the voltmeter, $IV_1$ the current in the measurement mesh and $R_{\text{internal}}$ the inner electrical resistance of the voltmeters ($6^{\text{th}}$ order of magnitude, MΩ).

![Circuit diagram](image)

(a) Circuit diagram

![Equivalent](image)

(b) Equivalent

**Figure 2.5:** Sketch of the circuit diagram and equivalent circuit diagram for the four–point method (Based on drawings from [5]).

Equaling the first two equations of (2.9) yields $IV_1$. The result put in the third equation of (2.9) gives $U_1$

$$ IV_1 = \frac{IR_{\text{sample}}}{R_1 + R_2 + R_{\text{internal}} + R_{\text{sample}}} \Rightarrow U_1 = R_{\text{sample}} I(1 - \alpha) \quad (2.10) $$

with

$$ \alpha = \frac{R_1 + R_2 + R_{\text{sample}}}{R_1 + R_2 + R_{\text{internal}} + R_{\text{sample}}} = \left(1 + \frac{R_{\text{internal}}}{R_1 + R_2 + R_{\text{sample}}} \right)^{-1} \ll 1 \quad (2.11) $$
As long as the inner electrical resistance of the voltmeters is large compared to the sum over the ohmic resistance of the sample, contacts and cables — what holds true under normal conditions — in a good approximation the equation for $U_1$ in (2.10) reads:

$$U_1 = R_{\text{sample}} I$$

(2.12)

For the conventional two-point method the measurement would have given

$$U_1 = I \cdot (R_3 + R_4 + R_{\text{sample}}).$$

(2.13)

By this for a small ohmic resistance of the sample the measurement would have shown a too large drop in voltage. Here, a better choice is the four-point method that offers an enhancement.
Chapter 3

Simulations

Different simulations have been performed, whose features and properties will be analyzed.

3.1 Sunrays

The computer program Sunrays 1.0 is a ray tracing program for three–dimensional simulation of solar cells with different cell materials, surface textures, multilayer ARCs, encapsulations, geometries for illumination and illumination spectra. Additionally the polarization of the incident light can be fully taken into account. For the ray tracing the geometrical optics is combined with the complete solution of the Maxwell’s equation at dielectric coated interfaces. A Monte–Carlo model simulates the effects of the polarization of individual photons. A sufficient statistic can be achieved for mixed polarization for a large number of calculated beam paths. The program includes a data bank of optical parameters of different materials that easily can be extended by adding data if there is the need for. The generation profile of charge carrier pairs is calculated in dependence from the cell thickness by Sunrays. The raw data can be processed by programs like Origin or PC–1D (simulation program for the electrical device properties) and depicted in graphics. That way one obtains information about the properties of certain cell parameters, for example like the reflectivity of a back surface coating or the thickness of a BSR. The computer simulation program Sunrays also offers the possibility to simulate the surface properties of different materials by a constant Lambert factor for all wavelengths. The Lambert factor can be continuously set from total directional to completely diffuse characteristics.

3.2 Results from the Sunrays simulation

By anticipation, that all calculation performed by Sunrays have been performed under the assumption of normal incident light to obtain the maximum efficiency of irradiation and to reduce the computational time. The program Sunrays has great advantages in the simulation of different textures to improve the light trapping. The aim is to enlarge the effective path length of light in the cell by a special geometry respectively to trap the light completely and therefore to increase the probability of absorption for charge carrier generation by the amount of passes. Obviously the program had problems in calculation with the choice of a flat surface because of easy recognizable errors. For example a silicon solar cell without texture pattern but with an ARC at 600 nm did not show the expected minimum in reflectance close to 600 nm. The result of the simulation however could be used qualitatively, because the wavelength range above 1 micron was the region of interest in that case. In special these were the simulations named “Solarzelle_01” and “Solarzelle_03”. The associated graphics are attached to the appendix B. Because of the tremendous computation time and the program incompatibility towards newer and faster computers, a detailed search for the error reason has been resigned. The problem did not occur for uncoated materials and texturated cells. Sunrays also revealed an enormously disadvantage by not being able to calculate the internal quantum efficiency. That means even if the light trapping geometry is improved the program does not allow access to any information about the change of charge carrier generation in the solar cell at a certain wavelength range. A clue for probable enhancements was provided by the simulations
named “Solarzelle_02” and “Si_Wafer”. They give a clue for the front surface properties of a cell to have a small directional dependency in transmission. In relation to the front surface properties, the backside should have a larger directional fraction in reflectance to optimize the light trapping in the cell and to suppress the contribution to the total reflectivity of the backside.

3.3 Optics

Within the scope of a masters thesis [6] the computer simulation program “Optik” has been developed. The program is capable to calculate and plot the reflectance and transmittance graphs for given optical constants $n$ and $k$. Vice versa it determines $n$ and $k$ from the measured $R$ and $T$ data in dependence of the wavelength. In addition, parameters like the layer thickness or an assumption for the surface roughness are required. Mono- and double layer systems can be handled under the assumption of the materials to show interference effects or not. A detailed description of the mathematical and technical programming details is described elsewhere [6]. The formulas used for the calculation of the reflectance and transmittance have been explicitly calculated in a general form and are given in section 4.1.
Chapter 4

Basics of optics

4.1 Reflectance– and transmittance coefficients

The goal is to calculate the reflectance $R$ and the transmittance $T$ of a crystal or rather of coplanar layers. For the sake of simplicity all media should be homogeneous, isotropic, surfaces and interface junctions ideally flat and non-lambertian. Top and bottom layer are assumed to be semi-infinite. Starting point for the calculation are Maxwell’s equations (MKS-system, [7]):

$$
\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0 \quad \nabla \cdot \mathbf{D} = \rho
$$

$$
\nabla \times \mathbf{H} - \frac{\partial \mathbf{D}}{\partial t} = \mathbf{j} \quad \nabla \cdot \mathbf{B} = 0
$$

(4.1)

To solve them for the field strengths, the so-called material equations are introduced:

$$
\mathbf{D} = \epsilon \cdot \mathbf{E} = \epsilon_0 \cdot \mathbf{E} + \mathbf{P}
$$

$$
\mathbf{B} = \mu \cdot \mathbf{H} = \mu_0 \cdot \mathbf{H} + \mathbf{M}
$$

(4.2)

$\mathbf{E}$ and $\mathbf{H}$ are the corresponding field strengths (in Volts and Ampere per meter respectively). $\mathbf{D}$ is the electric and $\mathbf{B}$ the magnetic induction, $\mathbf{M}$ is the magnetic and $\mathbf{P}$ the electric polarization. $\rho$ denotes the electric space charge density and $\mathbf{j}$ the electric current density. The dielectricity $\epsilon$ and permeability $\mu$ are tensors of rank 2 and can be considered as scalar parameters in isotropic media and independent from the field strengths (At the high field strengths of a focused laser for example non-linear effects occur, i.e. the dependencies of $\epsilon$ and $\mu$ of the field strengths are not longer negligible.). $\epsilon_0$ is the dielectric constant and $\mu_0$ the permeability constant of the particular fields in free space. They are exact by definition. By use of the Gauss’ and Stokes’ integral theorem one obtains the conditions for continuity for the normal components of $\mathbf{E}$ and $\mathbf{B}$ (discontinuity in the tangential components of $\mathbf{H}$ and $\mathbf{D}$) in relation to the interfacial area in the common case.

Figure 4.1: Reflectance and transmittance at an interface in a cross section through the plane of incidence. Modified from [6].

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In figure 4.1 the indices of $k$ stand for the incident ($i$), reflected ($r$) and the transmitted ($t$) wave vector. The angle of incidence equals the angle of reflectance ($\vartheta = \vartheta'$). By the conditions of continuity one obtains Snell’s refractive law:

$$\frac{\sin(\vartheta)}{\sin(\vartheta')} = \frac{n_1}{n_0}, \quad (4.3)$$

and furthermore the Fresnel’s formulas:

$$r_\perp = \frac{n_0 \cos \vartheta - n_1 \cos \vartheta'}{n_0 \cos \vartheta + n_1 \cos \vartheta'} \quad t_\perp = \frac{2n_0 \cos \vartheta}{n_0 \cos \vartheta + n_1 \cos \vartheta'}, \quad (4.4)$$

$$r_\parallel = \frac{n_1 \cos \vartheta - n_0 \cos \vartheta'}{n_1 \cos \vartheta + n_0 \cos \vartheta'} \quad t_\parallel = \frac{2n_0 \cos \vartheta}{n_1 \cos \vartheta + n_0 \cos \vartheta'}$$

In equation (4.4) $r_\perp$, $t_\perp$, $r_\parallel$ and $t_\parallel$ are the reflectance and transmittance coefficients respectively for the vector of the electric field strength component polarized normal to the plane of incidence. $n$ denotes the refractive index and is labelled by the number of the corresponding medium. $t_\perp$ and $t_\parallel$ are always positive. That is the reason for the propagation of transmitted wave without phase shift.

The reflected wave shows a different behavior: If $n_0 < n_1$ is valid, then $r_\perp$ is negative, i.e. the perpendicular component has a phase shift by $\pi$. The parallel component does this only for $\vartheta + \vartheta' < \pi/2$ by $\pi$ (Condition for Brewster’s angle).

If $n_0 > n_1$ is true, the behavior of the phases becomes more complicated. $r_\perp$ is persistent positive, but shows for angles exceeding the angle of total internal reflection ($\vartheta_c = \arcsin(n_1/n_0)$) a continuously phase shift between 0 and $\pi$. The exact value requires a numerical analysis for the corresponding refractive indices. $r_\parallel$ is negative in the region of $\vartheta + \vartheta' < \pi/2$ and therefore has a phase shift by $\pi$. For $\pi/2 \leq \vartheta + \vartheta' < \vartheta_c$, $r_\perp$ is positive and by that there is no phase shift. But from $\vartheta_c$ on there is, similar to $r_\parallel$, a continuous phase shift. This phase shift is exploited for example in ARCs by putting destructive interference into the condition for the incident and the inside the medium reflected, back travelling wave.

For normal incidence there is no need for distinction between the two polarizations. In addition the formulas become symmetrical for the medium in relation to the entrance and exit and can be redefined in a more simple sense to:

$$r = r_\perp = -r_\parallel = \frac{n_0 - n_1}{n_0 + n_1} \quad t = t_\perp = t_\parallel = \frac{2n_0}{n_0 + n_1} \quad (4.5)$$

If the medium absorbs, the refractive index becomes a complex number $n^*$:

$$n^* = n + i \cdot k \quad (4.6)$$

The intensity $R$ of the reflected respectively the transmitted light $T$ are given by:

$$R = |r|^2 = \frac{(n_0 - n_1)^2 + (k_0 - k_1)^2}{(n_0 + n_1)^2 + (k_0 + k_1)^2} \quad (4.7)$$

$$T = 1 - R$$
4.2 Monolayer system

For the calculation of the total reflectivity or the total transmittance respectively of a thin coplanar layer of thickness $d$ and refractive index $n_1$ sandwiched between two media with $n_0$ and $n_2$, one can do the following illustration (see figure 4.2):

![Figure 4.2: Multi–beam interference of a simple layered coplanar system. Modified from [6].](image)

For reasons of an easy survey the course of the beams is sketched obliquely — for the calculation normal incidence is assumed. The formulas can be obtained from summing over all individual rates of $r$ and $t$. In addition to this the absorption and the change of the phase within the layer has to be taken into account. For a single pass of the wave through the layer of thickness $d$ the amplitude of the field is damped by the factor

$$\exp \left(-\frac{2\pi kd}{\lambda}\right)$$

and its phase is altered by means of the optical path length about

$$\Delta \varphi = \frac{2\pi nd}{\lambda}$$

These effects are also taken into consideration by multiplying the amplitude of the field of the plane waves by the factor $\exp(i\delta)$.

$$\delta = \frac{2\pi d(n + i \cdot k)}{\lambda} = \frac{2\pi dn^*}{\lambda}$$

For the coefficients of reflectance and transmittance a more clear notation is introduced: $r_{ij}$ and $t_{ij}$, which denote the corresponding interfacial crossing between the different media. In this case the light would be reflected at the interface from medium $i$ to medium $j$ respectively transmitted. By help of the Stokes’ relations (4.11)

$$r_{ij} = -r_{ji}$$
$$t_{ij} = -t_{ji}$$
$$1 = t_{ij}r_{ji} - r_{ij}r_{ji}$$

one obtains by summation and conversion of the constituent parts a geometric series, whose limit for $r$ and $t$ reads:

$$r = \frac{r_{01} + r_{12}e^{2i\delta}}{1 + r_{01}r_{12}e^{2i\delta}}$$
$$t = \frac{t_{01}t_{12}e^{i\delta}}{1 + r_{01}r_{12}e^{2i\delta}}$$

(4.12)
Finally, reflectance $R$ and transmittance $T$ are given by

$$ R = |r|^2 \quad T = \left| \frac{n_0^*}{n_2^*} \right| \cdot |t|^2 $$

(4.13)

For the numerical evaluation one has to deal with real terms admittedly. A conversion for the expressions of $R$ and $T$ yields explicitly to:

$$ R = \frac{(u_1^2 + v_1^2)e^{\alpha d} + 2(u_1u_2 + v_1v_2)\cos(\beta d) + 2(u_2v_1 - u_1v_2)\sin(\beta d) + (u_2^2 + v_2^2)e^{-\alpha d}}{(u_3^2 + v_3^2)e^{\alpha d} + 2(u_3u_4 + v_3v_4)\cos(\beta d) + 2(u_4v_3 - u_3v_4)\sin(\beta d) + (u_4^2 + v_4^2)e^{-\alpha d}} $$

(4.14)

$$ T = \frac{16(n_1^2 + k_1^2)(n_0^2 + k_0^2)(n_2^2 + k_2^2)}{(u_3^2 + v_3^2)e^{\alpha d} + 2(u_3u_4 + v_3v_4)\cos(\beta d) + 2(u_4v_3 - u_3v_4)\sin(\beta d) + (u_4^2 + v_4^2)e^{-\alpha d}} $$

using the abbreviations:

$$ u_1 = (n_0 - n_1)(n_1 + n_2) - (k_0 - k_1)(k_1 + k_2) \quad v_1 = (n_0 - n_1)(k_1 + k_2) + (n_1 + n_2)(k_0 - k_1) $$

$$ u_2 = (n_0 + n_1)(n_1 - n_2) - (k_0 + k_1)(k_1 - k_2) \quad v_2 = (n_0 + n_1)(k_1 - k_2) + (n_1 - n_2)(k_0 + k_1) $$

$$ u_3 = (n_0 + n_1)(n_1 + n_2) - (k_0 + k_1)(k_1 + k_2) \quad v_3 = (n_0 + n_1)(k_1 + k_2) + (n_1 + n_2)(k_0 + k_1) $$

$$ u_4 = (n_0 - n_1)(n_1 - n_2) - (k_0 - k_1)(k_1 - k_2) \quad v_4 = (n_0 - n_1)(k_1 - k_2) + (n_1 - n_2)(k_0 - k_1) $$

(4.15)

$$ \alpha = \frac{4\pi k_1}{\lambda} \quad \beta = \frac{4\pi n_1}{\lambda} $$

If the layer is of adequate thickness $d$ compared to the wavelength $\lambda$, there are no interference effects. That means for a multiple reflection one does not have to care about the phase and can add up to all the reflected and transmitted intensities respectively. In an analogous procedure, with respect to

$$ R_{ij} = R_{ji} \quad T_{ij} = T_{ji} $$

(4.16)

one obtains:

$$ R = R_{01} + \frac{T_{01}^2 + R_{12}e^{-2\alpha d}}{1 - R_{01}R_{12}e^{-2\alpha d}} \quad T = \frac{T_{01}T_{12}e^{-\alpha d}}{1 - R_{01}R_{12}e^{-2\alpha d}} $$

(4.17)

The coefficients $R_{ij}$ and $T_{ij}$ can be calculated pursuant the preceding considerations.
Double layer system

The situation is comparable to the monolayer system:

\[
\begin{array}{c|ccc}
\text{air} & 0 \\
\text{film} & n_1 + ik_1 & 1 \\
\text{substrate} & n_2 + ik_2 & 2 \\
\text{air} & & & 3
\end{array}
\]

Figure 4.3: Coplanar double layer system. Modified from [6].

Now, there are two absorbing layers of which only the top is assumed to show interference effects. The layer 2 (substrate, thickness \(d_2\)) is therefore supposed to be very thick compared to the upper layer 1 (film, thickness \(d_1\)). The calculation is performed as follows: Firstly one specifies \(R\) and \(T\) for the system 0–1–2, named \(R_{02}\), \(R_{20}\), \(T_{02}\) and \(T_{20}\). Afterwards the coefficients are put into the formulas for \(R\) and \(T\) for the system 0–2–3, which does not show interference in layer 2. Explicit follows:

\[
\begin{align*}
R_{02} &= \frac{(u_1^2 + v_1^2)e^{\alpha_1 d_1} + 2(u_1 u_2 + v_1 v_2) \cos(\beta d_1) + 2(u_2 v_1 - u_1 v_2) \sin(\beta d_1) + (u_2^2 + v_2^2)e^{-\alpha_1 d_1}}{(u_2^2 + v_2^2)e^{\alpha_1 d_1} + 2(u_3 u_4 + v_3 v_4) \cos(\beta d_1) + 2(u_4 v_3 - u_3 v_4) \sin(\beta d_1) + (u_4^2 + v_4^2)e^{-\alpha_1 d_1}} \\
R_{20} &= \frac{(x_1^2 + y_1^2)e^{\alpha_1 d_1} + 2(x_1 x_2 + y_1 y_2) \cos(\beta d_1) + 2(x_2 y_1 - x_1 y_2) \sin(\beta d_1) + (x_2^2 + y_2^2)e^{-\alpha_1 d_1}}{(x_2^2 + y_2^2)e^{\alpha_1 d_1} + 2(x_3 x_4 + y_3 y_4) \cos(\beta d_1) + 2(x_4 y_3 - x_3 y_4) \sin(\beta d_1) + (x_4^2 + y_4^2)e^{-\alpha_1 d_1}} \\
T_{02} &= \frac{16(n_1^2 + k_1^2)\sqrt{(n_0^2 + k_0^2)(n_2^2 + k_2^2)}}{(u_1^2 + v_1^2)e^{\alpha_1 d_1} + 2(u_3 u_4 + v_3 v_4) \cos(\beta d_1) + 2(u_4 v_3 - u_3 v_4) \sin(\beta d_1) + (u_4^2 + v_4^2)e^{-\alpha_1 d_1}} \\
T_{20} &= \frac{16(n_1^2 + k_1^2)\sqrt{(n_0^2 + k_0^2)(n_2^2 + k_2^2)}}{(x_1^2 + y_1^2)e^{\alpha_1 d_1} + 2(x_3 x_4 + y_3 y_4) \cos(\beta d_1) + 2(x_4 y_3 - x_3 y_4) \sin(\beta d_1) + (x_4^2 + y_4^2)e^{-\alpha_1 d_1}}
\end{align*}
\]

whereat the further abbreviations are (by anticipation of \(\alpha_2\)):

\[
\begin{align*}
x_1 &= (n_2 - n_1)(n_1 + n_0) - (k_2 - k_1)(k_1 + k_0) ; \\
y_1 &= (n_2 - n_1)(k_1 + k_0) + (n_1 + n_0)(k_2 - k_1) \\
x_2 &= (n_2 + n_1)(n_1 - n_0) - (k_2 + k_1)(k_1 - k_0) ; \\
y_2 &= (n_2 + n_1)(k_1 - k_0) + (n_1 - n_0)(k_2 + k_1) \\
x_3 &= (n_2 + n_1)(n_1 + n_0) - (k_2 + k_1)(k_1 + k_0) ; \\
y_3 &= (n_2 + n_1)(k_1 + k_0) + (n_1 + n_0)(k_2 + k_1) \\
x_4 &= (n_2 - n_1)(n_1 - n_0) - (k_2 - k_1)(k_1 - k_0) ; \\
y_4 &= (n_2 - n_1)(k_1 - k_0) + (n_1 - n_0)(k_2 - k_1)
\end{align*}
\]

\[
\alpha_1 = \frac{4\pi k_1}{\lambda} ; \quad \alpha_2 = \frac{4\pi k_2}{\lambda}
\]

Now the coefficients are put into the second subsystem, as mentioned before:

\[
R = \frac{R_{02} T_{02} R_{20} R_{23} e^{-2\alpha_2 d_2}}{1 - R_{02} R_{20} R_{23} e^{-2\alpha_2 d_2}} \quad T = \frac{T_{02} T_{20} R_{23} e^{-\alpha_2 d_2}}{1 - R_{02} R_{20} R_{23} e^{-\alpha_2 d_2}}
\]

with the coefficients:

\[
R_{23} = \frac{(n_2 - n_3)^2 + (k_2 - k_3)^2}{(n_2 + n_3)^2 + (k_2 + k_3)^2} \quad T_{23} = 1 - R_{23}
\]
The calculation of $T_{23}$ is done that way, because an analogous equation with the Fresnel’s coefficients is only true for real refractive indices (and angles). For the special case that the media 0 and 3 are air ($n_{0,3} = 1$ and $k_{0,3} = 0$) the formulas and abbreviations given above simplify to:

$$
\begin{align*}
    u_1 &= (1 - n_1)(n_1 + n_2) + k_1^2 + k_1 k_2 ;
    v_1 &= (1 - n_1)(k_1 + k_2) - k_1(n_1 + n_2) \\
    u_2 &= (1 + n_1)(n_1 - n_2) - k_1^2 + k_1 k_2 ;
    v_2 &= (1 + n_1)(k_1 - k_2) + k_1(n_1 - n_2) \\
    u_3 &= (1 + n_1)(n_1 + n_2) - k_1^2 - k_1 k_2 ;
    v_3 &= (1 + n_1)(k_1 + k_2) + k_1(n_1 + n_2) \\
    u_4 &= (1 - n_1)(n_1 - n_2) - k_1^2 + k_1 k_2 ;
    v_4 &= (1 - n_1)(k_1 - k_2) - k_1(n_1 - n_2) \\
    x_1 &= (n_2 - n_1)(n_1 + 1) + k_1^2 - k_1 k_2 ;
    y_1 &= (n_2 - n_1)k_1 + (n_1 + 1)(k_2 - k_1) \\
    x_2 &= (n_2 + n_1)(n_1 - 1) - k_1^2 - k_1 k_2 ;
    y_2 &= (n_2 + n_1)k_1 + (n_1 - 1)(k_2 + k_1) \\
    x_3 = u_3 ;
    y_3 = v_3 \\
    x_4 = u_4 ;
    y_4 = v_4
\end{align*}
$$

(4.22)

and

$$
T_{02} = T_{20} = \frac{16(n_1^2 + k_1^2)\sqrt{(n_2^2 + k_2^2)}}{(u_3^2 + v_3^2)e^{\alpha_1 d_1} + 2(u_3 u_4 + v_3 v_4)\cos(\beta d_1) + 2(u_4 v_3 - u_3 v_4)\sin(\beta d_1) + (u_4^2 + v_4^2)e^{-\alpha_1 d_1}}
$$

(4.23)

For the case that the top thin layer of material 1 should not show any interference effects at all, one obtains:

$$
\begin{align*}
    R &= R_{02} + \frac{T_{02}T_{20}R_{23}e^{-2\alpha_2 d_2}}{1 - R_{02}R_{23}e^{-2\alpha_2 d_2}} \\
    T &= \frac{T_{02}T_{23}e^{-\alpha_2 d_2}}{1 - R_{02}R_{23}e^{-2\alpha_2 d_2}}
\end{align*}
$$

(4.24)

with

$$
\begin{align*}
    R_{02} &= R_{01} + \frac{T_{01}T_{10}R_{12}e^{-2\alpha_1 d_1}}{1 - R_{01}R_{12}e^{-2\alpha_1 d_1}} \\
    T_{02} &= \frac{T_{01}T_{12}e^{-\alpha_1 d_1}}{1 - R_{01}R_{12}e^{-2\alpha_1 d_1}} \\
    R_{20} &= R_{21} + \frac{T_{21}T_{12}R_{10}e^{-2\alpha_1 d_1}}{1 - R_{10}R_{21}e^{-2\alpha_1 d_1}} \\
    T_{02} &= T_{20}
\end{align*}
$$

(4.25)

and

$$
\begin{align*}
    R_{01} &= R_{10} = \frac{(n_0 - n_1)^2 + (k_0 - k_1)^2}{(n_0 + n_1)^2 + (k_0 + k_1)^2} \\
    T_{01} &= T_{10} = 1 - R_{01} \\
    R_{12} &= R_{21} = \frac{(n_1 - n_2)^2 + (k_1 - k_2)^2}{(n_1 + n_2)^2 + (k_1 + k_2)^2} \\
    T_{12} &= T_{21} = 1 - R_{12} \\
    R_{23} &= \frac{(n_2 - n_3)^2 + (k_2 - k_3)^2}{(n_2 + n_3)^2 + (k_2 + k_3)^2} \\
    T_{23} &= 1 - R_{23}
\end{align*}
$$

(4.26)

whereby for the special case, medium 0 and 3 are just air ($n_{0,3} = 1$ and $k_{0,3} = 0$), $R_{01}$ and $R_{23}$ can be furthermore simplified to:

$$
\begin{align*}
    R_{01} &= \frac{(1 - n_1)^2 + k_1^2}{(1 + n_1)^2 + k_1^2} \\
    R_{23} &= \frac{(n_2 - 1)^2 + k_2^2}{(n_2 + 1)^2 + k_2^2}
\end{align*}
$$

(4.27)
4.4 Multilayer system and matrix method

For an increasing number of layers the equations grow in size and their calculation becomes more complicated. To cope with that problem one can apply the matrix method. The advantages of this method are in particular a simple processing by a computer and the application to periodic structures e.g. dielectric Bragg mirrors that can be used in laser resonators as frequency selective mirrors. For layered systems like an ARC multilayers consisting of a number of layers greater than two the method becomes vital for the reasons mentioned before. The 2x2 matrix method is adequate for homogeneous and isotropic multilayer systems but for anisotropic systems matrices of higher dimensionality are needed. Because this method is a generalization of the problem treated before it will be explained in short terms and the proceeding elucidated.

Figure 4.4: The situation in a coordinate system.

A plane electromagnetic wave that incites under an angle \( \Theta \) to the surface normal of a flat interface of two dielectric media can be written in general of the form:

\[
E = \begin{cases} 
(E_1 e^{-i k_1 r} + E'_1 e^{-i k'_1 r}) e^{i \omega t} & x < 0, \\
(E_2 e^{-i k_2 r} + E'_2 e^{-i k'_2 r}) e^{i \omega t} & x > 0
\end{cases}
\]

\[ H = \frac{1}{\mu \omega} \cdot (k \times E) \quad (4.28) \]

is a solution for the two wave equations

\[
\nabla^2 E - \mu \epsilon \frac{\partial^2 E}{\partial t^2} = 0 \quad \nabla^2 H - \mu \epsilon \frac{\partial^2 H}{\partial t^2} = 0, \quad (4.29)
\]

whose follow from Maxwell’s equations for \( E \) and \( H \). The wave is decomposed in two different polarizations: s–waves (TE)have only \( E \)-field components normal to the plane of incidence and p–waves (TM) only \( E \)-field components parallel. The continuity condition yields an equation system (Annotated thereby is that these are put under the additional assumption of vanishing surface current and surface charge carrier densities. A situation that is convenient for many areas of optical problems [7].) The equation system can be written in a matrix form that describes the changes in the field amplitudes. For that reason they are called dynamic matrices. Written in full they read:

\[
D_s(i) = \begin{pmatrix} 1 & 1 \\
1 \cos \Theta_1 & -n_1 \cos \Theta_1 \end{pmatrix} \quad ; \quad D_p(i) = \begin{pmatrix} \cos \Theta_1 & \cos \Theta_1 \\
n_1 & -n_1 \end{pmatrix} \quad (4.30)
\]

The index \( i \) denotes the corresponding medium. The indices \( s \) and \( p \) stand for the appropriate polarization. The crossing from medium \( i \) to medium \( i + 1 \) is given by the transition matrix

\[
D_{s,p}(i, i + 1) = D_{s,p}^{-1} D_{s,p}(i + 1) \quad (4.31)
\]
This transition matrix can be formally written as

\[ D(i, j) = \frac{1}{t_{ij}} \begin{pmatrix} 1 & r_{ij} \\ r_{ij} & 1 \end{pmatrix}. \]  

(4.32)

where the distinction between the different polarizations is denoted by the Fresnel’s coefficients \( (r_{ij}, t_{ij}) \). The propagation matrix \( P(j) \) accounts for the transition of layer \( j \) by the wave:

\[ P(j) = \begin{pmatrix} e^{i\phi_j} & 0 \\ 0 & e^{-i\phi_j} \end{pmatrix} ; \quad \phi_j = k_{j,x}d_j \]  

(4.33)

A system that consists of a number of \( N \) layers is written in general as:

\[ \begin{pmatrix} A_0 \\ B_0 \end{pmatrix} = D_0^{-1} \cdot \left[ \prod_{i=1}^{N} D(i) \cdot P(i) \cdot D^{-1}(i) \right] \cdot D_S \cdot \begin{pmatrix} A'_S \\ B'_S \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \cdot \begin{pmatrix} A'_S \\ B'_S \end{pmatrix} \]  

(4.34)

with

\[ r = \frac{M_{21}}{M_{11}} \quad t = \frac{1}{M_{11}} \quad \text{and} \quad R = \frac{M_{21}^2}{M_{11}^2} \quad ; \quad T = \frac{n_S \cos \Theta_S}{n_0 \cos \Theta_0} \cdot \frac{1}{|M_{11}|^2} \]  

(4.35)

The index 0 refers to the medium in front of the \( N \) layers and the index \( S \) (substrate) the medium behind. \( A \) and \( B \) are the amplitudes of the plane wave. For an absorbing media the refractive index becomes a complex number. So the validity area of the formulas is restricted to lossless media 0 and \( S \) otherwise the wave vectors and angles could also become complex numbers and the calculation is no longer thoroughly correct.

From the mathematical properties of the matrices different theorems can be demonstrated for this method such as the principle of reversibility and energy conservation. These are not just of theoretical interest, but they also do not contain any new insights.

### 4.5 Application of a back surface reflector

If the absorption is set equal to zero in the formula (4.17) at the end of section 4.2 for \( R \) without interference the reflectivity amount of the backside can be varied for a given constant reflectivity of the front surface \([8]\). A plot of this calculation is given in the figure below:

![Figure 4.5: Total reflectance over back surface reflectivity.](image-url)
By that it becomes obvious that by a preferably high reflectivity at the backside in consequence also a high total reflectance is followed. The reflectance of the backside is dependent on its surface properties i.e. the appearance of the material at the interface. The simulations by Sunrays parameterized this behavior by the Lambert factor (diffuse/directional).

4.6 Loss minimizing

Initially a short survey on the optical losses of silicon solar cells will be given. The losses are caused by:

a) Reflectance of the front surface

One or more ARCs can minimize it. From the formulas for layered systems the conditions follow for layer thickness ($\lambda/4$) and refractive index (For example: If a single layer $i$ should act as an ARC, $n_i = \sqrt{n_{i-1}n_{i+1}}$ must be true).

b) Shadowing effects by the metal grid on the surface

This effect is reducible by circa 33% for upwards–tapered contact fingers whereby the reflected light at this point can be in–coupled. Number and width of the contact fingers have to be optimized in relation to the electrical resistance of the layer of the solar cell.

c) The absorption of the long wavelengths of the sunlight is too poor in the region of the band gap. The probability of absorption can be increased by enlargement of the optical path of the light length inside the crystal. This is called optical confinement and light trapping. It will be explained in the following.

For directional reflection under an angle of $0^\circ$ to the normal of the surface no inner total reflection is possible for a light confinement inside the material what can be seen from a simple calculation. A method to cope with that problem is to provided the backside with a diffuse reflectance:

![Figure 4.6: Reflectance behavior for a lambertian backside [9].](image)

Only light inside the hatched part (cone) of the in figure 4.6 can exit the material. The angle $\Theta_c$ can be calculated from the condition for total internal reflection:

$$\sin \Theta_c = \frac{1}{n}$$  \hspace{1cm} (4.36)

For an averaged real refractive index of 3.5 for silicon, this angle becomes $17^\circ$ and the corresponding radiation loss is about 8.5% [10]. Technically a flat surface is realizable by an extremely fine polish or a rough surface by selective directional etching of the crystal as an additional process step of a fabrication. The etching can also be used to make a chemical texture that leaves small more or less randomly distributed pyramids on the surface. A mechanical texture would be for example V–grooves. A surface texture is another possibility to increase the optical path length inside the material.

Simple geometric considerations for the condition of the critical angle of total internal reflection give rise to provide the front and back of a solar cell with V–grooves which are twisted by $90^\circ$ to
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Figure 4.7: Beam course for a texturated surface for the example of Si [9].

each other. Further advantage of this proceeding is its economy. The concept is already in use. A calculation to the structure above shows a reduction from 35% to 10% of the total reflectance [9]. This can be diminished by an ARC layer down to 3% (Coating by: vacuum deposition, spin coating or screen printing). More information about different geometries of textures are described elsewhere [11] and it is pointed out that the depth of the grooves should be larger than the diffusion length of the minority charge carries whereby the efficiency of collecting these charge carriers is increased.

To draw a conclusion, the light should be trapped inside the cell and increase the probability of absorption for the generation of electron–hole–pairs by multiple reflection. If absorption is also taken into account, the parameters \( R \) and \( T \) get reduced because of the relation:

\[
R + T + A = 1
\]  

(4.37)

Details on the different absorption mechanisms and their importance will be given in section 5.5.
In this chapter deals with the physical properties of silicon that are relevant for the studies. The focus is set on crystal properties, the energy states and the optical properties in special the different processes of absorption.

5.1 Polycrystalline silicon

The ingot casting process reduces costs compared to an extensive crystallizing process when a huge directed monocrystal is fabricated. The molten silicon is cooled down under control in a rectangular graphite pot so that the grain boundaries arrange themselves columnar i.e. normal to the surface. Grain boundaries that would be directed parallel to the p–n interface later might have a heavy parasitic impact because they are recombination centers of the free charge carriers. The emerging structure is crystalline coarse. The crystallites are in the order of mm up to cm. The bulk material is cut into quadratic slices of 300 – 400 micron thickness, which have an area of 10x10 cm\(^2\) up to 30x30 cm\(^2\). These Si wafers are the raw material for solar cells. Grain boundaries and defects are the preferred routes for diffusion of impurity atoms like hydrogen\(^1\) (H) and phosphorous\(^2\) (P) in the technical fabrication process. The technical fabrication process also requires a p-type ground doping with boron (B) in the order of 10\(^{16}\) cm\(^3\). The boron doping negligibly affects the optical properties like index of refraction and therefore absorption [12].

5.2 Energy states, density of states and the Fermi level

The occupation of allowed energy states by charge carriers (electrons and defect electrons (= holes)) of a particular band depends on the temperature. It is also affected by the spin because of Pauli’s

\(^1\)Hydrogen can also be ion implanted. The Si becomes passive because the H–atoms saturate the free (dangling) bonds. The exact mechanism of the process is not yet fully understood.

\(^2\)Example of a n-doping (gettering): An existing phosphate–silicate layer binds during the diffusion process a large amount of impurities. These travel to the surface during the diffusion process and can be afterwards etched off.
principle. The statistical behavior of the principle of choice finds its expression in the Fermi–Dirac distribution function $f(E)$ (5.1),

$$f(E) = \frac{1}{1 + \exp \left( \frac{E - E_F}{k_B T} \right)}$$  \hspace{1cm} (5.1)

which gives the occupation probability of an energy level $E$ (see figure 5.2).

![Figure 5.2](image)

**Figure 5.2**: Fermi–Dirac distribution function [9].

In figure 5.2 $E_F$ is the Fermi energy, $k_B$ denotes Boltzmann’s constant and $T$ is the absolute temperature in Kelvin. The Fermi energy is defined for an occupation probability of 50% in an intrinsic (ideal and pure) semiconductor at $T = 0$ K and is in the middle of the band gap i.e. between the valence band and the conduction band.

For electrons for the example the density of states determines the number of electrons $N(E)$ (5.2) in the conduction band $E_C$ for a small energy range $dE$. Thereby the electrons are assumed to be free i.e. there is no interaction due to external fields. By assigning an effective mass $m^*_e$ interaction concerning the crystal lattice is taken into account. The electrons are identified by charge and in the frame of Heisenberg’s uncertainty principle this leads to

$$N(E) \cdot dE = \frac{8\pi \sqrt{2} (m^*_e)^{3/2}}{h^3} \sqrt{E - E_C} \cdot dE$$  \hspace{1cm} (5.2)

where $h$ is Planck’s constant.

![Figure 5.3](image)

**Figure 5.3**: Number of allowed states as a function of energy $E$. 
The characteristics of the allowed states is plotted in figure 5.3. The curve above $E_C$ concerns the electrons and the the curve below $E_V$ the holes. The effective density of states is expressed by

$$n = \int_{E_C}^{\infty} f(E) \cdot N(E) \cdot dE.$$  \hfill (5.3)

I.e. the number of electrons per volume unit in the conduction band is an integral over energy of the product density of states times probability distribution function. For an intrinsic semiconductor at a finite temperature the integral is easy to approximate. The calculation is transferable for the effective density of states of the holes (with an effective mass $m_p^*$) in the valence band yielding to the equation:

$$n = 2 \cdot \left( \frac{2\pi m_n^* k_B T}{\hbar^2} \right)^{3/2} \cdot \exp \left( \frac{E_F - E_C}{k_B T} \right) \quad \text{and} \quad p = 2 \cdot \left( \frac{2\pi m_p^* k_B T}{\hbar^2} \right)^{3/2} \cdot \exp \left( \frac{E_V - E_F}{k_B T} \right).$$  \hfill (5.4)

In equilibrium the intrinsic charge carrier density $n_i$ is:

$$n_i^2 = n \cdot p \quad ; \quad n = p$$ \hfill (5.5)

Temperature and doping shift the equilibrium of $n$ and $p$ as well as the Fermi level.

5.3 Calculation of the ionization degree

The systematic introduction of certain impurity atoms into a neat semiconductor is called doping. In this work, silicon was doped with aluminium. The aluminium is alloyed into the backside forming a $p^+$ like electrical contact that is also at the same time a BSF and a BSR. The superscript plus indicates high doping. In comparison to this the basis has a relative low $p$–type ground doping of boron in the order of $10^{16}$ cm$^{-3}$. It is negligible for the considered high Al doping of $10^{18}$ cm$^{-3}$. The condition of neutrality in the equilibrium is given in equation (5.6). 

---

3By screen printing: An aluminium paste is printed on the reverse side and alloyed in a furnace at 800°C (eutectic temperature: 577°C). After recrystallization a $p^+$–doping remains (The doping level depends on the solid–state solubility which is a function of temperature). The Al excess is separated as a mixture of Al and Si whose consistence (circa 12% Si in Al) corresponds to the situation for alloying at the eutectic temperature.
\[ n + n_A^- = p \quad \text{with} \quad n_A^- = \frac{n_A}{1 + g_A \cdot \exp \left( \frac{E_A - E_F}{k_B T} \right)} \]  

(5.6)

In equation (5.6) \( n_A^- \) denotes the thermally ionized density of acceptors, \( n_A \) the corresponding density of their total number, \( g_A \) the associated degeneration factor for the spin and \( E_A \) the distance from the acceptor energy level to the valence band edge energy, which is set to 0 eV for practical reasons. The entire equation is written as:

\[
2 \cdot \left( \frac{2\pi m^*_p k_B T}{\hbar^2} \right)^{3/2} \cdot \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\sqrt{X} \cdot dX}{\exp \left( X - \frac{E_F - E_C}{k_B T} \right) + 1} = \frac{n_A}{1 + g_A \cdot \exp \left( \frac{E_A - E_F}{k_B T} \right)} + 1
\]

(5.7)

Equation (5.7) determines the Fermi level. The integrals occurring in this equation are called Fermi integrals. In this case the Fermi level is located at 0.0767 eV (In the calculation the band structure is neglected.) — slightly above the acceptor level at 0.057 eV. If \( E_F \) might be smaller than \( E_V \) or greater than \( E_C \), the Fermi level would be degenerated. According to Sommerfeld’s degeneration criterion

\[
p_{\text{critical}} = \frac{1}{3\pi^2} \left( \frac{2\pi m^*_p k_B T}{\hbar^2} \right)^{3/2}
\]

(5.8)

the doping level however is below the critical doping confirming the result for the location of the acceptor level given above. The value can be used to calculate the ratio of ionized to neutral acceptors:

\[
\frac{n_A^-}{n_A} = \frac{1}{1 + g_A \cdot \exp \left( \frac{E_A - E_F}{k_B T} \right)}
\]

(5.9)

For an estimated value of \( g_A = 2 \), it is about 52%. The band structure takes the spin–orbit coupling into account and the maximum of the valence band edge is twofold degenerated (i.e. \( g_A = 4 \) [13,14]). For this reason the result for the Fermi level is 0.0831 eV and 41% for the degree of ionization. The interest in the degree of ionization is based on the changes in the electrical conductivity and therefore the connected optical properties like absorption due to free charge carriers.

From an analogous calculation of a \( p^{++} \)-doping with boron at the reverse side (acceptor level at 0.045 eV), which is used for BSFs, a Fermi energy of 0.0787 eV and an ionization degree of 48% follow. Room temperature (\( T = 300 \) K) has been assumed in the calculation.
5.4 Optical properties of silicon

Electrons in a crystal lattice can be described by periodic wave functions. This characterization allows to calculate the eigenenergy states which yield the band structure dependant on the momentum. The band structure is in common only plotted for the first Brillouin zone because of the lattice periodicity (see figure 5.5).

![Figure 5.5: First Brillouin zone [11].](image)

Several methods exist to calculate the band structure. In addition the phonon dispersion curves i.e. the possible vibrational modes of the crystal respectively the first Brillouin zone can be calculated.

![Figure 5.6: Phonon dispersion curves of silicon [11].](image)

5.5 Absorption

The absorption is described by the absorption coefficient $\alpha$ and depends on the wavelength $\lambda$. The relation between $\alpha$ and $k$ of the complex refractive index has been explained in section 4.1 and 4.2. Now the different mechanisms of absorption firstly will be elucidated for intrinsic silicon.

5.5.1 Phonon assisted absorption

The transition from the valence band maximum to the minimum of the conduction band requires a certain minimum energy and change in momentum $\Delta k$, because the initial and the final state do not have an equal $k$. The momentum of a photon is negligible small and therefore at least of one phonon is needed.
Physical properties of silicon

Figure 5.7: Energy band scheme of silicon in the first Brillouin zone [11].

Figure 5.8: (a) Two possible transitions. (b) Scheme for the energy and momentum conditions (The phonon energies are sketched exaggerated [11]).

In figure 5.8 (a) two different ways for an initial state $a$ and a final state $c$ are sketched. The way $a \rightarrow b \rightarrow c$ the electron has a direct virtual transition $a \rightarrow b$ by absorption of a photon of lower energy as the band gap and goes immediately from $b$ to $c$ under absorption or emission of a phonon that has the required momentum. Figure 5.8 (b) gives the conditions of energy and momentum conservation for an indirect transition. The required phonon energy is given by:

$$h\nu = E_{\text{initial}} - E_{\text{final}} - E_P.$$  \hfill (5.10)

In figure (5.10) $h\nu$ is the photon energy and $E_P$ the phonon energy. For phonons the Bose–Einstein statistic is valid:

$$f_B = \frac{1}{e^{\frac{E_P}{k_B T}} - 1}. \hfill (5.11)$$

The absorption coefficient is calculated of a product of the Bose–Einstein statistic, a constant and the integral of the product of the density of states of initial and final state from the initial to the final energy (Details on the calculation are given in [13]). The indices $a$ and $e$ distinguish between absorption and emission. The final result for $\alpha$ is given by:

$$\alpha = \alpha_a + \alpha_e = \frac{A(h\nu - (E_G - E_P))^2}{e^{\frac{E_P}{k_B T}} - 1} + \frac{A(h\nu - (E_G + E_P))^2}{1 - e^{-\frac{E_P}{k_B T}}}. \hfill (5.12)$$
$E_G$ is the band gap energy, i.e. the difference between the valence and conduction band energies. For silicon at room temperature, in a good approximation $E_G$ is given by [9]:

\[
E_G(300 \text{ K}) = 1.17 \text{ eV} - \frac{2.9 \cdot 10^{-4} \text{ eV} \cdot T^2}{T + 167 \text{ K} + \frac{31.8 \text{ K}}{T}} \bigg|_{T=300 \text{ K}} \approx 1.1 \text{ eV} \tag{5.13}
\]

The calculation of the constant $A$ is more of theoretical interest and results from a tedious calculation involving time dependent perturbation theory [15]. The constant $A$ is characterized by a $(h\nu)^{-1}$ dependency that does not vary much in the region of the band edge. The square frequency dependence of $\alpha$ is really interesting. It can be experimentally observed in the range between 0.6 and 1.05 micron. The absorption coefficient $\alpha$ becomes larger for smaller wavelength.

5.5.2 Absorption edge

The absorption process involves the charge carriers electrons and holes which attract each other. They can bind to a lattice site or move as a free exciton through the crystal. Their binding energy can be estimated by use of the hydrogen model. Therefore the dielectric constant of silicon and the reduced mass $m_r^*$ (normalized to the rest mass of the electron) of the effective masses of the corresponding charge have to be put into equation (5.14):

\[
E_{\text{exciton}}[\text{eV}] = -\frac{13.6 \cdot m_r^*}{\epsilon_\text{Si}^2 \cdot s^2} ; \quad \frac{1}{m_r} = \frac{1}{m_n^*} + \frac{1}{m_p^*}. \tag{5.14}
\]

The natural $s$ labels the state of the exciton. M. Green [11] and Ch. Kittel [16] calculate a value of 14.7 meV for the ground state ($s = 1$). Higher values for $s$ are not observed under normal conditions, because they are in the absorption edge. Excitons modify the behavior of absorption by forming steps that can be identified by the phonon energies involved in the absorption process. At very low temperatures the phonon absorption processes are strongly suppressed what can be seen from the Bose–Einstein distribution. Hard to recognize in the experiment are very small peaks in the absorption spectrum at 1.17 eV and 1.21 eV originating from phonon emission processes. These correspond to TA and TO phonons at energies of 18.3 meV and 57.8 meV respectively. The 40 meV difference corresponds to the distance between the small peaks.

![Absorption edge for pure silicon](image)
The absorption spectrum hides fine structures at increasingly higher temperatures. The investigation of these becomes admittedly complicated because the effects are very small. If $\alpha$ comes close to zero the fundamental absorption processes fade out. But the possibility of one or multi phonon processes suggests to exploit wavelengths above 1.2 micron by light confinement. The idea is to enlarge the optical path by an increase of the number of to and fro cycles of the light inside the cell. Although the absorption is weak, the enlarged optical path increases the probability of absorption. M. Green [11] denotes for this purpose some involved relevant numbers: The band gap at 1124.2 meV, the absorption edge assisted by a phonon at 1051.7 meV respectively by two phonons at 987 meV, the Raman phonon (optical phonon in the center of the zone) at 64.7 meV, the TO phonon at 57.8 meV and the exciton at 14.7 meV.

5.5.3 Urbach’s rule

Additional absorption below the band gap $E_G$ can occur due to an extrinsic effect: The perturbation of the lattice periodicity e.g. by a defect or impurities (dopings) yields to additional states at the border of valence and conduction band (see figure 5.10).

Urbach himself empirically found a rule that expresses the excess absorption $\Delta \alpha$:

$$\frac{1}{E} = \frac{1}{k_B T} = \frac{d \ln(\Delta \alpha)}{d(h\nu)}.$$  \hspace{1cm} (5.15)

5.5.4 Direct absorption

Silicon has a direct band gap at 3.4 eV (see the energy band scheme in figure 5.7). For the corresponding wavelengths smaller than 380 nm, this results in a huge increase of the absorption coefficient.
An absorption coefficient larger than $10^6 \text{ cm}^{-1}$ means that 99% of these wavelengths are absorbed in the upper 10 nm of the silicon. The slow decrease of $\alpha$ for wavelengths greater than 380 nm can be explained by indirect absorption processes for example at the indirect gap at point L in $k$–space (see figure 5.7). Indeed this is not an argument for the observed strength, but can be rather explained from an enhancement of the one and two phonon processes in general, if the absorbed photon energy comes closer to the energy of a direct transition. The reflectance spectrum of silicon contains information about the strong direct absorption process. There are peaks for the photon energies at 3.4 eV, 4.5 eV and 5.7 eV. These correspond to so–called critical points in $k$–space where the gradients of valence and conduction band are equal. Critical points are points of high symmetry like the zone center Γ and the face center L. Critical points also exist along lines of high symmetry like Λ, Δ and Σ (see figure 5.5).

5.5.5 Absorption by free charge carriers and the lattice

The absorption process due to free charge carriers and the lattice does not generate electron–hole pairs. Between photons and phonons of the lattice there is only interaction for wavelength around 10 micron, because of the required energy and momentum conservation and the relatively weak phonon energies. For free charge carriers there is a distinction between interband absorption with initial and final energy states in different bands and intraband absorption whose states are within the same band. The absorption strength depends on temperature and doping.

\[ \alpha = \frac{\mu e^2 n}{4\pi\epsilon_0 c^3 m^* \eta} \left( \frac{1}{\tau_m} \right) \sim \lambda^2 \]  

In equation (5.16) $\mu$ is the free charge carrier mobility, $n$ the density of the free charge carriers, $e_0$ the elementary charge unit, $c$ the speed of light in vacuum, $\eta$ the real part of the refractive index according to Drude’s theory and $\tau_m$ the momentum relaxation time. The slight increase in the

Figure 5.12: Absorption coefficient ($T = 300 \text{ K}$) of n–type Si for dopings in units of $10^{17} \text{ cm}^{-3}$ and height of the band edge as a function of charge carrier concentration [18].

On the left figure 5.12 shows a rise of the absorption coefficient of n–type silicon at room temperature for an increase in doping. On the right, the absorption peaks are plotted over the charge carrier concentration. For the weak doped samples in figure 5.12 a structure is revealed in the range between 6 and 20 micron which can be attributed to absorption of the lattice and impurities, mainly due to oxygen. For the highly doped samples there is a linear range for the region greater than 5 micron, which originates of intraband absorption due to free charge carriers. This agrees with the classical theory ($\lambda^2$ dependency, Drude’s formula):

\[ \alpha = \frac{\mu e^2 n}{4\pi\epsilon_0 c^3 m^* \eta} \left( \frac{1}{\tau_m} \right) \sim \lambda^2 \]  

In equation (5.16) $\mu$ is the free charge carrier mobility, $n$ the density of the free charge carriers, $e_0$ the elementary charge unit, $c$ the speed of light in vacuum, $\eta$ the real part of the refractive index according to Drude’s theory and $\tau_m$ the momentum relaxation time. The slight increase in the
range from 2 to 4 micron for all dopings originates from the intraband absorption of the two lowest conduction bands in X (see figure 5.7). An similar increase does not appear in the case of a p-type doping but in fact there is a strong $\lambda^2$ dependency that can be observed in the region up to the band edge. In the far infrared (FIR) there is a structure, which arises from interband absorption in the valence band. An increase in the doping level means an increase of the imaginary part of the refractive index. The absorption process (free charge carriers) is the same like for metals which is responsible for the high reflectivity in the VIS [11].

5.5.6 Temperature dependency

The temperature dependency pointed out in section 5.5.1 concerns not only the energy band gap but energy bands in general. Close to room temperature the energy of the indirect band gap in silicon can be linear approximated by

$$E_G(T) = 1.206 - 0.000273 \cdot T.$$  \hspace{1cm} (5.17)

Thus at higher temperatures also photons of lower energy are involved in electron–hole pair generation. In addition the direct band gap decreases for an increase in temperature. This becomes particularly clear for wavelengths greater than 400 nm.

Figure 5.13: Absorption coefficient of pure Si dependent on temperature. From [18].

For solar cells however this increase is not sufficient enough to compensate the destructive impacts of temperature on the open circuit voltage and the filling factor.

5.5.7 Additional effects of absorption

Some more effects linked to absorption are given in short and qualitatively:

- The Franz–Keldysch effect found in 1958 shifts the band edge by influence of a large electric field because the lattice translation invariance no longer valid. This effect is not significant [11, 19, 20].

- The Burstein–Moss shift is a displacement of the absorption edge. It occurs for high charge carrier concentrations like for high dopings (larger than $10^{18} \text{ cm}^{-3}$ [21]). So the Fermi level is in the valence or conduction band respectively (degeneration). In special this effect becomes
large if the mobility of one charge carrier respectively its effective mass is significantly greater than its opposite. This is due to a multi body effect of interactions between the charge carriers and the randomly distributed doping atoms, which constrict the band gap and therefore make it smaller.

- Scattering of charge carriers at acoustic and optic phonons is also possible as well as at ionized doping atoms. This can be noticed of the power law of absorption as a function of the wavelength. Different and even contradictory results for highly doped Silicon are not unusual as it is stated by different authors. This was also a result from an extensive literature research. There are too many different parameters for the doping. Every situation requires its own differentiation of the occurring effects.

- $\alpha$ is also a function of an external magnetic field, because it can shift and split energy levels. For most semiconductors a decrease of $E_G$ can be noticed by application of increasing pressure. The decrease of $E_G$ has an impact on the electrical resistance and thereby these semiconductors are of interest for strain gauges in technical application. Of physical interest is the fact that by applying pressure gives rise to more complex circumstances because the bands can overlap and change the nature of the fundamental band gap. Another alternative to change the band gap and thereby the absorption behavior is chemical modification like alloying. In addition for these mixed crystals the lattice constant can be varied. Examples for it the quasi–binary compounds $Ga_xIn_{1-x}As_yP_{1-y}$ and $Al_xGa_{1-x}As_ySb_{1-y}$ can be taken.

5.6 Effects of doping with respect to generation and recombination of charge carriers

The general treatise of the basics from this topic is tedious and complicated hence only a qualitative summary will be given. Starting point is Poisson’s equations for the electrical field in a dielectric medium and the two continuity equations for the charge carriers. Effects like tunnelling or charge transport by hopping afford modifications respectively another continuity equation.

5.7 Generation of charge carriers

The charge carrier generation rate depends on the irradiated photon flux and is reduced due to by parasitic and generation processes. The spectral distribution of the photon flux requires an integration over the different wavelengths. In addition the cross section, the concentration and occupation probability of the lower states have to be taken into account. The generation rate is reduced by recombination. Photons of energy greater than 3.5 eV can excite electron–hole pairs by impact ionization. This is a negligible small effect.

The possibility to bring defect states in the middle of the band gap was considered to become an excitation process in two steps for exploiting the photons of lower energy. Admittedly the enhancement in optical absorption is overshadowed from the parasitic electrical properties of these states because they strongly recombine (see section 5.8.3) the different charge carriers. This application would only be favorable for concentrator solar cells, which have an excellent optical confinement. Technical possibilities have to be improved therefore.

5.8 The different kinds of recombination

5.8.1 Radiative recombination

This process is the inversion of absorption: The electrons fall back from the conduction band to the valence band by annihilation of the same number of holes. The recombination energy corresponds directly to the distance between the bands. For Silicon absorption and recombination have the same probability, therefore the lifetime of the charge carriers should be appropriately long for indirect semiconductors. The effect has an inferior position and depends on the doping concentration.
5.8.2 Auger recombination

The situation of the Auger effect is described as follows: An electron in the conduction band recombines with a hole in the valence band and transfers the freed energy to another electron in the valence band which is excited to a higher level and relaxes by many impacts back to its initial state. For this process a lifetime can be defined which has a proportional dependency on charge carrier concentration. The analogous process to the electron–electron–hole process described above is the electron–hole–hole process. But the lifetime is for that process negligible short and therefore has an inferior position.

5.8.3 Recombination induced by impurity trap states

Basically in a semiconductor impurity trap states determine the recombination of charge carriers. Depending on the position of the band gap they are called deep or shallow trap states. A theory for this recombination process has been developed in 1950 by W. Shockley, W. Read and R.N. Hall.

![Figure 5.14: Recombination by trap states. Image source: [9].](image)

For an energy level $E_T$ between valence band $E_V$ and conduction band $E_C$ there are four fundamental processes possible:

1. electron capture from the conduction band of an unoccupied energy level,
2. emission of an electron of an occupied energy level into the conduction band,
3. capture of a hole from the valence band from an occupied energy level,
4. emission of a hole into an unoccupied state in the valence band.

For the calculation of the probability for the particular process the following assumptions are taken, which are mostly true:

- there should be no other transitions between the different levels,
- the position of an energy level does not depend on its charge state,
- the time of emission and capture is short compared to the average of the elapsed time between capture and emission process,
- the density of trap states $N_T$ is small compared to the doping concentration.

The recombination rate $R$ (in $[s^{-1} \text{cm}^{-3}]$) can be expressed by

$$R = \frac{v_{th} N_T (n p - n_i^2)}{\left( \frac{1}{\sigma_p} \right) \cdot (n + n_i) + \left( \frac{1}{\sigma_n} \right) \cdot (p + p_i)}$$  \hspace{1cm} (5.18)
Thereby is
\[ \nu_{th} = \text{the thermal velocity} \]
\[ n = \text{the electron concentration in the equilibrium} \]
\[ p = \text{the hole concentration in the equilibrium} \]
\[ N_T = \text{the density of the trap levels} \]
\[ \sigma_n = \text{the capture cross section of the electrons} \]
\[ \sigma_p = \text{the capture cross section of the holes} \]
\[ E_T = \text{the energy of the impurity level} \]
\[ n_1 = n_i \cdot \exp \left( \frac{E_T - E_i}{k_BT} \right); \quad p_1 = p_i \cdot \exp \left( \frac{E_i - E_T}{k_BT} \right) \] (5.19)

For the lifetime of the charge carriers
\[ \tau = \frac{\Delta n}{R} \text{ with } \Delta n = np - n_i^2 \] (5.20)
is introduced. Two different cases are distinct:

1. High injection: The number of excess charge carriers is much higher than the number of carriers due to background doping. Both of the energy bands have enough charge carriers and basically their lifetime depends on the capture probability and not on concentration.

2. Low injection: The concentration of the background doping is much higher than the concentration of excess charge carriers. As a result the lifetime of the corresponding minority charge carriers is inverse proportional to the number of impurity trap states. The energy levels in the middle of the band gap have the most reducing character and lifetime there is independent from doping, whereas for shallow impurity trap states the dependency of lifetime strongly depends on doping (hyperbolic cosine dependency).

### 5.8.4 Recombination due to doping

Adding up the recombination processes, the total lifetime can be written as:
\[ \frac{1}{\tau_{\text{total}}} = \frac{1}{\tau_{\text{radiation}}} + \frac{1}{\tau_{\text{Auger}}} + \frac{1}{\tau_{\text{trap}}} \] (5.21)

Every process is a more or less strongly doping dependent. The according theoretical curves are summarized and plotted in figure 5.15. Auger recombination is considered to gain importance for doping concentrations larger than \(10^{18} \text{ cm}^{-3}\).

For the range from \(10^{16}\) up to \(10^{18} \text{ cm}^{-3}\) there are significant discrepancies between theory and experiment [9]. In the citation several authors are named, who worked on that subject. A makeshift is the empirically determined relation after Kendall:
\[ \tau = \frac{\tau_0}{1 + \frac{N_{\text{doping}}}{7 \cdot 10^{15}}} \] (5.22)

Thereby the charge carrier lifetime \(\tau_0\) of pure undoped Silicon is assumed to be 400 µs.
Figure 5.15: Lifetime as a function of doping concentration [9].
The Cary 5 spectral photometer was used to measure reflectance and transmittance spectra of different silicon samples. All of the samples were of orientated monocrystalline silicon of different p–type boron ground doping levels.

<table>
<thead>
<tr>
<th>Sample No.</th>
<th>Thickness in µ (micron)</th>
<th>Ohmic resistivity Ωcm</th>
<th>Calculated doping</th>
<th>Annotation</th>
<th>Degree of ionization</th>
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</thead>
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<td>505</td>
<td>0.0122</td>
<td>5.50 · 10⁻¹⁸</td>
<td></td>
<td>24.3%</td>
</tr>
<tr>
<td>wafer 1</td>
<td>450–575</td>
<td>0.005–0.025</td>
<td>1.95 · 10⁻¹⁹</td>
<td>manufacturers' information</td>
<td></td>
</tr>
<tr>
<td>wafer 2</td>
<td>510</td>
<td>0.0165</td>
<td>3.45 · 10⁻¹⁸</td>
<td></td>
<td>29.7%</td>
</tr>
<tr>
<td>wafer 3</td>
<td>505</td>
<td>0.0141</td>
<td>4.39 · 10⁻¹⁸</td>
<td></td>
<td>26.8%</td>
</tr>
<tr>
<td>wafer 4</td>
<td>535</td>
<td>12000</td>
<td>1.10 · 10⁻¹²</td>
<td>manufacturers' information</td>
<td></td>
</tr>
<tr>
<td>wafer 4</td>
<td>500–550</td>
<td>2000–4000</td>
<td>3.32 · 10⁻¹²</td>
<td></td>
<td>100%</td>
</tr>
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<td>0.53</td>
<td>3.03 · 10⁻¹⁶</td>
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<td>94%</td>
</tr>
<tr>
<td>fragment 2</td>
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<td>3.04 · 10⁻¹⁶</td>
<td></td>
<td>94%</td>
</tr>
<tr>
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<td>1.57</td>
<td>9.32 · 10⁻¹⁵</td>
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<td>98%</td>
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<tr>
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<td>1.40 · 10⁻¹⁶</td>
<td></td>
<td>97%</td>
</tr>
</tbody>
</table>

Table 6.1: Survey of the investigated silicon samples

Each sample thickness in table 6.1 was mechanically determined by a micrometer screw and the results from measurements at different places averaged. The samples seemed to be of homogeneous thickness (largest difference: 5 micron). The ohmic resistivity was determined by a four–point ohmmeter that was built for special purposes at the chair of Prof. Dr. Bucher. The measurement of wafer no.4 turned out to be a problem because it had an extremely high ohmic resistivity due to its low doping level. The measurement required a different measuring head and high frequency voltage peaks and also the voltmeter and ammeter ranges had to be changed. The results are only equal in their order of magnitude. This is an indication that the measurement range of the device had been exceeded. In the following only the manufacturers’ information will be taken as relevant. The doping concentrations have been calculated by use of the computer program PC1D.

It takes about 20 minutes for the Cary 5 spectral photometer to warm–up at operational temperature. For long–term measurements the device could overheat. That could be observed in the measured curves because of strongly varying results. Possible standards for diffuse reflectivity there were four reflectors of 2%, 25%, 50% and 99% available to record a baseline for reflectance measurements. For the investigated silicon samples a baseline for 50% reflectivity has been recorded in the reflectance measurements. All measurements were performed in the wavelength range from 300 nm to 2500 nm in 5 nm steps. The sample chamber had to be closed tightly to avoid artifacts that stem from room light.

All transmission measurements used the same gauge (baseline). In addition to that a baseline of 100% (99%) reflectivity and of 0% transmission had to be recorded. For the latter the sample
beam was just blocked. Device internal the recorded baselines are used for error correction. For transmission measurements the samples had to be mounted in front of the Ulbricht sphere. It was necessary to pay attention on keeping the sample beam free to avoid measurement artifacts.

To get rid of the dust contamination on the sample surface, the wafer fragments were cleaned by use of neat ethanol and single use lens tissues. The wafers came directly from the fabrication process and were just taken out of their dust free carrier for the measurements. All of those were clean. For wafer no. 4 the manufacturers’ information was given that there were less than 20 particles of a size exceeding 300 nm on its surface. To estimate the amount of roughness of the single side polished samples (wafer no. 1–4), measurements have been performed on both sides. For the analysis of the data recorded two different ways were available:

1) The computer program “Optik” which calculates from the reflectance and transmittance data the values of $n$, $k$ and $\alpha$. The equations involved are two-dimensional and non-linear and can be solved by the Newton–Raphson iteration (roughly a two-dimensional Newton iteration). A problem was to find appropriate start values and a suitable number of mesh points, which also had to be fitted to certain wavelength ranges. Random checks gave the clue that this way would turn out to be inefficient and time wasting compared to another possibility:

2) The determination of the absorption coefficient $\alpha$ from the $R$ and $T$ equations for a thick coplanar slab without interference effects but absorption and multiple reflections inside. The equations required (see (4.17)) were given at the end of section 4.2. For the symmetric system air–silicon–air the reflectance coefficients $R_{ij}$ are also symmetric assuming normal incidence. Hence they are just denoted by $r$ in the following because they are also equal in value. This symmetry also holds true for the transmission coefficients and can be eliminated in the equations. Starting point is energy conservation equation (6.1).

$$R + T + A = 1$$  \hspace{1cm} (6.1)

A formal expression for the absorption $A$ can be obtained for the given equations $R$ and $T$:

$$R = \frac{r \cdot (1 + (1 - 2r) \cdot e^{-2\alpha d})}{1 - r^2 \cdot e^{-2\alpha d}}$$

$$T = \frac{(1 - r)^2 \cdot e^{-\alpha d}}{1 - r^2 \cdot e^{-2\alpha d}}$$

$$A = \frac{(1 - r) \cdot (1 - e^{-\alpha d})}{1 - r^2 \cdot e^{-2\alpha d}}$$  \hspace{1cm} (6.2)

The sample thickness is $d$. The equation for $R$ yields $r$. The obtained result is put into the equation for $T$. In turn, this equation is solved for $\alpha$. In total six equation result, pairwise identical. Out of the three remaining only one has a physical meaning:

$$\alpha = \frac{\ln \left(-\frac{1 + 2R - R^2 + T^2 - \sqrt{4T^2 + (1 - 2R + R^2 - T^2)^2}}{2T} \right)}{d}$$  \hspace{1cm} (6.3)

This equation allows to calculate the absorption coefficient $\alpha$ can be for recorded data of $R$ and $T$ at a certain wavelength and a given thickness $d$ of the sample substrate. Another consideration for the measured data is Beer’s law:

$$I(x) = I_0 \cdot e^{-\alpha x}$$  \hspace{1cm} (6.4)

The initial intensity $I_0$ is damped by the distance $x$ to $I(x)$ after entering a medium with absorption coefficient $\alpha$. Considering a wafer of 500 micron thickness, $\alpha$ has to be in the order of $10^3 \text{ cm}^{-1}$.
at least so that 30% (i.e. the amount of the primary reflection at the front surface) of the incident light from the front can exit again after a single reflection at the back. Figure 5.11 confirms this for wavelengths greater than 800 nm. That is the reason for an investigation of the reflectivity at the wafer backside starting from this wavelength is of interest. Plots of the analyzed data are shown in the figure 6.1 below.

Figure 6.1: (a) Square root of the absorption curve for silicon samples with different dopings. (b) Square root of the absorption coefficient of the fragment sample no. 4 in comparison to wafer no.4.

A linear trend for the wavelengths greater than 1.1 micron i.e. proportional to the band gap energy can be seen clearly for the doped samples apart from the low doped wafer no.4. The square root of \( \alpha \) is plotted. The linearity of the plot at a certain wavelength region confirms the quadratic \( \lambda \) dependency according to classic Drude theory, given in equation (5.16). According to the degree of ionization calculated in section 5.3, the absorption by free charge carriers for the NIR wavelengths seems to be feasible. The curves of the wafer fragment samples no.1 to 4 show nearly the same characteristics because their dopings are of equal amount. Therefore only one of the curves was picked out for representation and has been plotted. Calculated values for the absorption coefficient \( \alpha \) from the recorded data were at a wavelength of 1.25 micron, which corresponds to an energy of 0.99 eV, are compiled in table 6.2.

<table>
<thead>
<tr>
<th>Sample</th>
<th>No.</th>
<th>( \alpha ) [cm(^{-1})]</th>
<th>( \alpha^{1/2} ) [cm(^{-1/2})]</th>
<th>Reference in the literature</th>
<th>Source</th>
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</thead>
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<tr>
<td>wafer .......... 1</td>
<td></td>
<td>5.85 (5.32)</td>
<td>4.24</td>
<td>[21]</td>
<td></td>
</tr>
<tr>
<td>wafer .......... 2</td>
<td></td>
<td>5.41 (4.10)</td>
<td>3.54</td>
<td>[21]</td>
<td></td>
</tr>
<tr>
<td>wafer .......... 3</td>
<td></td>
<td>5.37</td>
<td>–</td>
<td>–</td>
<td></td>
</tr>
<tr>
<td>wafer .......... 4</td>
<td></td>
<td>0.23</td>
<td>0.49</td>
<td>–</td>
<td></td>
</tr>
<tr>
<td>fragment ....... 1</td>
<td></td>
<td>0.31</td>
<td>0.49</td>
<td>–</td>
<td></td>
</tr>
<tr>
<td>fragment ....... 2</td>
<td></td>
<td>0.30</td>
<td>0.29</td>
<td>–</td>
<td></td>
</tr>
<tr>
<td>fragment ....... 3</td>
<td></td>
<td>0.30</td>
<td>0.29</td>
<td>–</td>
<td></td>
</tr>
<tr>
<td>fragment ....... 4</td>
<td></td>
<td>0.31</td>
<td>0.31</td>
<td>–</td>
<td></td>
</tr>
<tr>
<td>( \alpha ) of pure Si ..</td>
<td></td>
<td>–</td>
<td>–</td>
<td>0.00</td>
<td>[22]</td>
</tr>
</tbody>
</table>

Table 6.2: Absorption coefficient \( \alpha \) calculated for various silicon samples

Although the wafer sample no.4 had a very high purity, its absorption coefficient deviates from the value of pure silicon what makes the comparison inconclusive but gives a hint for the increase of the absorption coefficient for an increase in doping. For comparison to references wafer no.1 had a doping of \( 5 \cdot 10^{18} \) cm\(^{-3}\) and for wafer no.2 \( 2.8 \cdot 10^{18} \) cm\(^{-3}\) were taken. In the first case the deviation is about 37% and in the second 53%. The estimated read off error for 2 mm from the graphs in the literature gives 1%. The method for calculation that has been used, differs from
Data analysis

Schmid’s [21]: The formula for $T$ has been resolved for $\alpha$ and the $r$ of pure Silicon has been used. The value calculated that way is given in brackets. Its deviation is about 25% and for wafer no.2 even lower, about 16%.

The deviations are reasonable for the following facts: The dopings of the samples compared are not equal. The baseline of the spectrometer corrected the reflectance measurement to a reference of 50% which is definitively too high. In addition there are possible errors due to the spectrometer because it is not an ideal measurement apparatus. For the measurements performed temperature has been neglected.

The constrictions for the literature reference were the following: the silicon had to be monocrystalline, the crystal orientated in (111) direction and predominantly doped with boron to a certain degree. The $R$–$T$ measurements had to be performed at room temperature. These restrictions reduced the number of published papers to only a few. The results of the different authors showed discrepancies. For the literature research the INSPEC database was used.

M. Green [23] gives an empirical formula for the absorption by free charge carriers:

$$\alpha_{\text{free carrier}} = 2.6 \cdot 10^{-18} n \lambda^3 + 2.7 \cdot 10^{-18} p \lambda^2$$ (6.5)

The expression for the $n$–type was left out in equation (6.5) because all samples had a $p$–type doping. The concentration of the ionized acceptors, which is the product of doping concentration and degree of ionization, is denoted by $p$. In analogy the same is valid for the $n$–type doping.

In figure 6.2 the degree of ionization is included. Only the free charge carriers, whose number in particular corresponds to the number of ionized doping impurities, contribute to absorption. The same way only the free charge carriers contribute to electrical resistivity measurement of a slab. Therefore one should keep in mind that in particular the total doping concentration is higher than the degree of ionization as it can be determined from by secondary ion mass spectroscopy (SIMS) measurement.

The BSF of a solar cell is about 10 micron thickness i.e. one way back and forth absorbs about 8% of the intensity in the wavelength range from 1 to 1.2 micron according to Beer’s absorption law. This loss is relevant for high efficiency solar cells whose BSFs have 96–98% reflectivity, but it can not be identified for industrial fabricated solar cells as a limit for charge carrier generation close to the band edge.

Figure 6.2: Comparison of the measured data from wafer no.1 to the empirical curve calculated from [23].
I want to express my kind gratitude to Prof. Dr. Bucher, whose lecture notes on the course “Solid-State Physics” and the elective courses “Introduction to Semiconductor Physics” and “Alternative Energies” have been proved in time to be very useful. I am also grateful to my supervisor Dipl.-Phys. Frank Huster, to Dr. Kristian Peter for his help and hints as well as all the other kind colleagues of the chair of Prof. Dr. Bucher, which lend me all the time their ear for my questions. A special thank goes to my colleague Dr. Ben Buchler for his help.
# Appendices

## Abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ARC</td>
<td>anti-reflection coating</td>
<td>1</td>
</tr>
<tr>
<td>BSF</td>
<td>back surface field</td>
<td>1</td>
</tr>
<tr>
<td>BSR</td>
<td>back surface reflector</td>
<td>1</td>
</tr>
<tr>
<td>FIR</td>
<td>far infrared</td>
<td>32</td>
</tr>
<tr>
<td>IR</td>
<td>infrared</td>
<td>1</td>
</tr>
<tr>
<td>LED</td>
<td>light emitting diode</td>
<td>6</td>
</tr>
<tr>
<td>min</td>
<td>minute</td>
<td>5</td>
</tr>
<tr>
<td>mm</td>
<td>millimeter (10⁻³ meter)</td>
<td>4</td>
</tr>
<tr>
<td>MΩ</td>
<td>Mega Ohms (10⁶ Ohm)</td>
<td>9</td>
</tr>
<tr>
<td>NIR</td>
<td>near infrared</td>
<td>3</td>
</tr>
<tr>
<td>nm</td>
<td>nanometer (10⁻⁹ meter)</td>
<td>4</td>
</tr>
<tr>
<td>PMT</td>
<td>photomultiplier tube</td>
<td>5</td>
</tr>
<tr>
<td>PTFE</td>
<td>polytetrafluoroethylene (Teflon)</td>
<td>7</td>
</tr>
<tr>
<td>SBW</td>
<td>spectral bandwidth</td>
<td>4</td>
</tr>
<tr>
<td>Si</td>
<td>silicon</td>
<td>v</td>
</tr>
<tr>
<td>SIMS</td>
<td>secondary ion mass spectroscopy</td>
<td>40</td>
</tr>
<tr>
<td>TE</td>
<td>transversal electric</td>
<td>19</td>
</tr>
<tr>
<td>TM</td>
<td>transversal magnetic</td>
<td>19</td>
</tr>
<tr>
<td>VIS</td>
<td>visible (light)</td>
<td>3</td>
</tr>
<tr>
<td>UV</td>
<td>ultraviolet (light)</td>
<td>3</td>
</tr>
</tbody>
</table>

Table A.1: List of abbreviations
Selected plots of the simulation results

The following plots are a selection of the results of the simulations performed with the program Sunrays. The plots were used to study the trends by variation of different cell parameters.

**Figure B.1: Simulation 01**
Selected plots of the simulation results

Figure B.2: Simulation 02
Figure B.3: Simulation 03
Figure B.4: Simulation 04
parasitary absorption

Figure B.5: Simulation 05
Selected plots of the simulation results

**Figure B.6**: Simulation 06
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