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On the Effect of Varying Spectral Conditions on Amorphous Silicon Solar Cell Performance

By

Christos Monokroussos

Doctoral Thesis
Submitted in partial fulfilment of the requirements for the award of
Doctor of Philosophy of Loughborough University

May 2011

© by Christos Monokroussos 2011
To my grandmother Calliope
(Στη γιαγιά μου Καλλιόπη)
Abstract

An opto-electrical modelling platform has been designed to model the effects of illumination spectra on amorphous silicon solar cells of different i-layer thickness and degradation state. The illumination spectra, which were investigated in this work, are solar simulator spectra and solar spectra recorded outdoors at CREST, Loughborough. These spectra are used to probe the effect of spectral variation on a-Si:H solar cell performance and its co-dependence with the state of the device.

For the case of indoor evaluation of performance of a-Si:H solar cells, it is shown that the performance of the device remains relative to the illumination source of the solar simulator. Spectra with Average Photon Energy (APE) higher than AM1.5G tend to overestimate the performance parameters ($J_{SC}$, MPP, $V_{OC}$) of the device, while spectra with APE lower than AM1.5G tend to underestimate the values of the performance parameters of the device. The maximum power deviation of most class-A solar simulators is less than 1% of the actual STC values, but the performance deviation may arise up to 4% for the case of LED light sources. It is suggested to apply voltage dependant corrections to the J-V characteristics, whenever the spectral mismatch between the illumination spectra and AM1.5G is significant.

The effects of outdoor spectral variation on the performance of a-Si:H solar cells has been investigated. The results show that light intensity is primarily responsible for a-Si:H outdoor performance. The APE of the outdoor spectra is also identified a significant factor for the variation of performance. The magnitude of maximum power deviations due to APE changes is in the range of ±3% as compared to power output of the device under the AM1.5G spectrum. The percentage of performance variation to STC differed for a-Si:H solar cells of different i-layer thickness and level of degradation. Specifically devices with thicker i-layer, which have suffered degradation, are prone to performance variations.

Finally, the energy yield and the performance ratio of amorphous silicon solar cells were reviewed in respect to outdoor spectral changes. The performance ratio is a useful method for cases where prediction of power output is necessary. However, it is suggested that PV modules should be rated on the basis of their annual energy yield, when possible.
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Chapter 1 – Introduction

Photovoltaic (PV) solar cells allow a direct conversion of light into electrical energy without any mechanical movement and pollution. In addition PV enjoy sufficient and nearly unlimited solar resources throughout the world. According to the British Petrol annual energy report the energy covering the world electricity generation in 2008 was estimated at 20,201.8TWh [1], while the United States Energy Information Administration (EIA) predicts a world need of 30TWh in 2030 [2]. Less than 0.33%¹ of the total available solar energy resources reaching earth’s crust in a year would be sufficient to cover the world energy needs in 2030. Despite their potential, solar photovoltaics at the moment are a small, but dynamically increasing segment of the energy market. Specifically, the total PV installed capacity rose to 13.4GW showing a dramatic increase of 70% in 2008 [3], which suffice to cover the 0.04% of the total electricity generation in 2008.

The increase of the PV installed capacity was naturally followed by an expansion of the PV industry production, which grew by a 66% in terms of megawatt production capacity during 2008 [3]. This increase reflected on both wafer based and thin-film solar cells, which are the two main sectors of the PV industry. The first currently dominate the PV market and are mainly polysilicon based technologies. The second include amorphous silicon (a-Si), copper-indium-gallium-diselenide (CIGS), cadmium telluride (CdTe) and organic cells based technologies, which have a lower production cost, but also lower conversion efficiency [4].

The major challenge facing solar electricity generation is the high associated cost per kWh compared to other energy technologies. This is a drawback which is especially true for wafer based technologies [4], as high deposition temperatures, the shortage of available polysilicon supplies [5] may result in wafer based module prices will remaining in place for the foreseeable future [7]. On the other hand thin-film technologies, which are currently being developed reduce the amount (or mass) of light absorbing material required in creating a solar cell. This can lead to reduced processing

¹ Assuming a conversion efficiency of 10%
costs compared to that of bulk materials. In addition, monolithic device design [8], use of inexpensive substrates [9], and manufacturing processes that are low temperature and possible over large areas are commonly used in the fabrication of main stream thin-film solar cells such as a-Si, CIGS and CdTe (eg. [10-12]. Independent energy analysts (such as [4], [5], [7]) predicted the cost per W\textsubscript{p} output of thin-film technologies to be 25% more competitive than wafer based technologies by 2010. For these reasons PV industry has shown a noticeable turn towards thin film technologies over the last five years. In 2004 the share of thin-film technologies on the total PV production in terms of MW barely exceeded 2.5%. Five years later thin-films jumped over 22% of the total production, as shown in Figure 1.

![Figure 1: Technology trends in PV production in terms of GW over the last five years. Data used in this graph were provided by IEA-PVPS [3].](image1)

Currently amorphous silicon thin-film technologies have a dominant market position comparing to CIGS and CdTe. In 2007 a-Si cell production capacity reached 53% of the total thin-film cell production [5], which is shown in Figure 2. Furthermore, the large majority of the thin-film installed capacity is a-Si photovoltaics [3]. Although the future is expected to be bright for all thin-film technologies, amorphous silicon shows the greatest potential for immediate installation. Analysts such as Duke et al. [13] who have ended a supply and demand analysis of the electricity market in the US suggest profitable selling price for amorphous silicon PV modules in a near-term time frame (2007–2016) is possible as long as module prices show a 40% decrease during the forthcoming decade. This is a realistic goal judging from the current module price

\footnote{The unit Watt-peak (W\textsubscript{p}) is by definition the power which a solar module yields at a “peak” irradiation of 1kW/m\textsuperscript{2} at standard test conditions (STCs). Standard test conditions are a set of reference photovoltaic device measurement conditions consisting of 1kW/m\textsuperscript{2} normally incident irradiance, 25°C module temperature and AM1.5 spectrum.}
trends; from 1998 to 2008 the cost per installed Watt had fallen by around 40% in IEA-PVPS countries\(^1\) [3].

![Proportional running capacities of thin-film technologies in 2009](image)

**Figure 2:** Proportional running capacities of thin-film technologies in 2009, based on data published by PV status report [5].

Hence, the initial challenge remains; would amorphous silicon photovoltaics expand in the market, the associated cost per kWh should be reduced. Many analysts, such as [13-15], agree that achieving this goal is but a simple task. While most recognise that any progress in the performance of a-Si technologies would have eventually to pass through cell, module and in the end system design, not so many pay attention to fundamental concepts of photovoltaic performance, which is the performance assessment itself.

At the moment, two principal quantities are used to characterise the output of photovoltaic systems. The first is the power rating, given by the efficiency of the PV module in a period of time over the efficiency of the same module under STCs [16]. The second is the energy yield, the actual electrical energy generated by the system in a given period of time [17].

\(^1\) The IEA-PVPS members in 2008 are: Australia, Austria, Canada, Denmark, EPIA, European Union, France, Germany, Israel, Italy, Japan, Korea, Malaysia, Mexico, the Netherlands, Norway, Portugal, Spain, Sweden, Switzerland, Turkey, the United Kingdom and the United States.
The efficiency of a device is strongly dependent upon the operating conditions under which it is evaluated. This has been understood for a long time and led to the standardisation of conditions for reporting laboratory-measured cell efficiencies, Standard Test Conditions (STC). This set of conditions provides common benchmarking for PV devices and is not only a research tool, but it is also the STC efficiency that is used to set the price of commercial modules in the marketplace. But, while PV modules are priced on the basis of their power rating, electricity consumers and suppliers buy and sell in units of energy.

In reality, most installed PV systems will rarely encounter conditions close to this standard. The irradiance not only will strongly vary according to the geographic location of the site (eg. as shown in Figure 3), but also with daily, annual and weather-based patterns. In practice high irradiances would also cause a raise in the module temperature to well over the STCs value. The solar angle of incidence naturally changes on a daily and annual basis and is rarely normal to the plane of the array. The irradiance spectrum also varies with solar position, as bulk attenuation in the atmosphere is highly wavelength-dependent and the path length changes with solar elevation. There is an additional dependence on the weather as cloud cover acts to further distort the spectrum. The extent of variation in realistic operating conditions and how far they are from STCs
is specific to the system location. Table I shows how frequently STCs were met in Loughborough, UK.

Table I: Matching between STCs and outdoor conditions at Loughborough, UK

<table>
<thead>
<tr>
<th>Condition</th>
<th>Percentage of Time Satisfied</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Module Temperature 25 ±2 ºC</td>
<td>8.8%</td>
</tr>
<tr>
<td>2. Irradiance 1000 ±50 Wm⁻²</td>
<td>2.9%</td>
</tr>
<tr>
<td>3. Spectrum AM1.5G ±0.1 eV</td>
<td>1.2%</td>
</tr>
<tr>
<td>4. Module Temperature 25 ±2 ºC, Irradiance 1000 ±50 Wm⁻²</td>
<td>0.1%</td>
</tr>
<tr>
<td>5. Module Temperature 25 ±2 ºC, Irradiance 1000 ±50 Wm⁻², Spectrum AM1.5G ±0.1 eV</td>
<td>0.0%</td>
</tr>
</tbody>
</table>

The chaotic nature of earth’s atmosphere is well-known, and one could expect a strong disparity between any specific set of conditions and the reality, which dynamically changes during the year and restricts calibrations to a limited number of times. For this reason module performance evaluation is carried out indoors, using standard steady-state, or pulse solar simulators that imitate the sun's light. Typical light sources used for this purpose are the quartz Xenon or Halogen lamps, modified by light filters to better match the solar spectrum. Recently LED solar simulators have gained momentum (e.g. [19]-[21]), but have not been commercialised yet. Solar simulators are classified to A, B and C according to their quality of spectral-match and light uniformity [22]. In general, solar simulators are viewed as cost effective tools, which allow rapid evaluation of PV modules. In reality, the light source may show a significant spectral mismatch and still be in accordance with the class A international standards [23], as shown in Table II. Therefore, indoor performance evaluation may be a laboratorially controlled, repetitive and precise method, but one should always keep in mind that its accuracy remains relative to the test conditions. Alternations in the test conditions and specifically the spectral conditions often occur in practice, and will result errors in the performance evaluation of the modules.
Table II: Average photon energy of commercialised solar simulators in the 350-1100nm region. The names of the solar simulators listed are not released due to confidentiality issues.

<table>
<thead>
<tr>
<th>Solar Simulator</th>
<th>Class</th>
<th>Average Photon Energy [eV]</th>
<th>Average Wavelength Difference to AM1.5G [nm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>#1</td>
<td>A</td>
<td>1.73</td>
<td>-39.83</td>
</tr>
<tr>
<td>#2</td>
<td>A</td>
<td>1.84</td>
<td>+2.28</td>
</tr>
<tr>
<td>#3</td>
<td>A</td>
<td>1.81</td>
<td>-6.92</td>
</tr>
<tr>
<td>#4</td>
<td>A</td>
<td>1.69</td>
<td>-58.85</td>
</tr>
<tr>
<td>#5</td>
<td>B</td>
<td>1.65</td>
<td>-75.30</td>
</tr>
<tr>
<td>#6</td>
<td>B</td>
<td>1.71</td>
<td>-49.16</td>
</tr>
<tr>
<td>#7</td>
<td>B</td>
<td>1.78&lt;sup&gt;1&lt;/sup&gt;</td>
<td>-20.46&lt;sup&gt;1&lt;/sup&gt;</td>
</tr>
<tr>
<td>#8</td>
<td>C</td>
<td>1.87</td>
<td>+11.16</td>
</tr>
<tr>
<td>Tungsten – 2800K</td>
<td>-</td>
<td>1.6</td>
<td>-100.07</td>
</tr>
</tbody>
</table>

The purpose of this thesis is to understand and assess the indoor and outdoor performance variation of amorphous silicon solar cells, due to changes in the excitation spectrum. In order to quantify these variations in performance one needs to model the specifics of a-Si devices, namely the device structure, which is a p-i-n junction rather than p-n junction, the wavelength dependent generation of electron-hole pairs and the effects of recombination, which in the case of a-Si is predominantly dangling-bond driven. The nature of dangling-bonds is especially important, as it is responsible for the metastability amorphous silicon exhibits, which is attributed to light-induced degradation. Amorphous silicon is known to increase the concentration of dangling-bonds, when exposed under a prolonged period in light radiation, an effect which is known as Staebler-Wronski Effect (SWE) [24]. This requires a simulation of the opto-electrical behaviour of the device, as this is the only way to accurately describe different combinations of excitation spectra and applied voltage. A synopsis of this thesis is briefly presented.

Chapter 2 describes the developed optical model. The model is designed to simulate the optical behaviour of a-Si solar cell devices with particular focus on the estimation of electron-hole generation profiles, as caused by different excitation spectra. A ray-tracing approach is followed, which allows the simulation of planar multi-layer optical structures with textured interfaces. The optical model is two-dimensional, treating light as propagating electromagnetic radiation.

<sup>1</sup> Solar Simulator #7 data are restricted in the 350-1000nm region. The spectral energy difference in respect to AM1.5G, in this case has also been restricted between 350-1000nm.
The development of an electrical model, which simulates the device physics of p-i-n junctions, is the subject of chapter 3. The model utilises the generation profiles calculated by the optical model and estimates the electron-hole collection at the terminals of the a-Si device in terms of current generation. Significant effort has been paid to accurately model the idiosyncrasies of a-Si devices, such as the varied electric field within the i-layer, dangling bond recombination and the level of degradation, which the device has suffered. The model is then validated in conjunction with the optical model presented in chapter 2 against experimental measurements.

In chapter 4 the effects of different spectra on the performance evaluation of amorphous silicon solar cells and its implications for the calibration are being examined. The aim is to understand the physical effects determining the uncertainty in the calibration process. Two effects are identified; first, the spectral mismatch between reference cells and the device, which is complicated significantly by the varying spectral response\(^1\) of the solar cell with applied voltage. Second, the fill factor of the device is affected by different spectra, increasing the measurement uncertainty significantly.

In chapter 5 the effects of seasonal and sky clearness variation on the performance of a-Si:H cells are investigated. It is shown that the efficiency under standard test conditions (STCs) is relative, as the actual efficiency of the cell may strongly vary. It is also shown that the deviation from STC efficiency depends on the light-management schemes of the cells, as well as the level of degradation of the device. It is concluded that, the optimisation and selection of devices based on their performance on standard test conditions in an non-degraded state may result in losses in the annual current generation and thus power.

Last but not least, it is imperative to understand that the future of photovoltaic evolution is directly linked to improvement of annual energy yield. However, this cannot happen only through material research and improved cell efficiencies, but also through a better understanding of indoors and outdoor photovoltaic performance assessment. The later is the topic of this thesis.

\(^{1}\) The spectral response of a PV material is the number of electron and holes collected at the device terminals per unit of photon energy.
Methodology

In this section the reasons of the approaches chosen to satisfy the aims of the thesis are being described. Specifically, research was conducted to determine the effects of the variation of spectral irradiation on the power evaluation of a-Si:H solar cells operating indoors and outdoors. So far the effects of spectral variation on a-Si:H performance have been studied experimentally and the effect has been understood qualitatively. However there has been no systematic attempt to model the effects of spectral variation to qualify such effects. The latter is the main goal of this thesis.

Research Objectives

Typical power evaluation of solar cells is carried out indoors using solar simulators, whose spectrum often varies significantly comparing to the standard AM1.5G. Moreover solar cells are made to operate outdoors, where the solar spectral irradiance is dynamically changing and is almost explicitly different than AM1.5G. Hence, the variation of spectral irradiance occurs in both indoor and outdoor conditions and thus, will affect the performance of the rated indoors and the energy yield of the operating outdoors a-Si:H solar cells. The purpose of this thesis is to quantify and assess the magnitude of such spectral effects on the performance of a-Si:H solar cells.

The effect of device state has also been part of the research objectives and especially its covariance with the variation of spectral irradiation. Currently devices of different i-layer thickness exist in the market, whose underlying performance may significantly change under different spectra. Additionally degradation, the aging of the devices, is also another crucial factor, which defines performance and is also affected by spectral effects. Therefore, in order to answer the question of what is the effect of spectral variation on performance, the state of the device should be examined simultaneously.

Detailing the Problem

The main problem, which needs to be answered, is how the effect of spectral variation could be quantified taking into account the state of the device in terms of current
generation. In fact, to resolve such a problem three sub-questions have to be answered separately.

1. How to evaluate the effect of different spectra on a-Si:H performance.
2. How to evaluate the effect of different device states on a-Si:H performance.
3. After assessing sub-questions 1 and 2, how could their co-dependence affect a-Si:H performance.

In order to answer the first question, the physics of photo-generation needs to be taken into account. Specifically, light of different wavelengths will be distributed differently within the device. Therefore, one needs to seek a platform, which will be able to analyse the optical distribution of light within a multi-layer structure, which is actually a thin film solar cell.
The second question can be answered as long as the statistics of carrier collection and regeneration are addressed considering the specifics of each device, such as different structures and defect densities. Hence, an electrical engine needs to be developed, which will evaluate the current density-voltage, $J$-$V$, characteristics of solar cell devices of different specifics.

The third question essentially refers to the way the two platforms would intercommunicate one with the other. This can be achieved as long as the output of the optical engine can be used as input in the electrical model in terms of generation rates.

**Research Design**

In this section the methods and its sequence applied to examine and quantify the problem of a-Si:H solar cell performance variation due to spectral effects will be presented. A synopsis of the research design is shown in Figure 4. A more detailed explanation of each step will be carried out later on.

The first step is to design two interacting models an optical and an electrical. This is essentially a holistic opto-electrical model, which will be able to take into account both the spectral irradiance and the state of the device. The second step is to validate the model. The validation will allow the correct examination of both spectral variation and state of the device and their co-dependence on the performance of the device. Having established and validated the model is required to place a solid basis, which will permit the quantification of the problem. In the following step the model will be used to examine different states of devices in both indoor and outdoor conditions.

**I. Development of the opto-electrical model**

The development of the opto-electrical model consists of two models, an optical and an electrical and is the basis for the work completed in this study. The optical model is able to calculate the spatial variation of photo-generation rate within a device based on the structural information of the device. The generation profiles are later used as input to evaluate the different spectral distributions and their underlying current generation. The electrical model should be able process different generation rate profiles and calculate the $J$-$V$ characteristics of different structures and device states. This is achieved by
using an in-depth semiconductor breakdown of the electric field distributions, the electron-hole carriers and their generation-recombination statistics within the device. In the final step the current flow is calculated based on the carrier populations.

**II. Validation and Calibration**

The developed model is calibrated based on three a-Si:H solar cell samples of different i-layer thickness; Cell 1 with i-layer thickness 250nm, Cell 2 with 400nm and Cell 3 with 600nm. The structural configuration and the used materials are known for all cells. The Cells 1, 2 and 3 are measured experimentally; their $J$-$V$ and $EQE$ characteristics are obtained under AM1.5G bias light. The opto-electrical model is then used to simulate the $J$-$V$ and $EQE$ characteristics of three theoretical cells of the same i-layer thickness and configuration with the sample cells Cell 1, 2 and 3. For the purpose of the simulations generic values in the typical range found in the bibliography are used. The theoretical results are then compared with the experimental measurements and a satisfactory agreement is achieved.

**Figure 5: Chart Flow of the Opto-Electrical Model Development**
III. Application of the model to quantify the effect of spectral variation on performance the problem

In the third step of the research design the opto-electrical model is used to evaluate the indoors and outdoors performance variations due to spectral mismatch between the actual light source and the AM1.5G spectrum. The investigation is applied on a system of six solar cells. Specifically, three i-layer thicknesses (250nm, 400nm and 600nm) and two degradation states (as-prepared and degraded), which vary only on their underlying defect density of amorphous silicon are selected.
Figure 7: Sketch of the methodology applied for the purpose of determining the indoor performance variation of a-Si:H solar cells as compared to the STC performance.

The indoor variation of performance deviation is probed using different light sources including A, B and C solar simulator spectra, Tungsten light source and LEDs. The combination of all light sources is examined on the system of all solar cells using the already developed opto-electrical model.

Figure 8: Sketch of the methodology applied for the purpose of determining the outdoor performance variation of a-Si:H solar cells as compared to the STC performance.

A similar approach is followed to quantify the magnitude of the outdoor variation of performance deviation due to spectral changes. In this case a complete set of annual spectral irradiance data is used as recorded at CREST, Loughborough, UK during 2003 and 2004. Again the data are applied on all II solar cells using the opto-electrical model.
IV. Application of the model to quantify the effect of spectral variation on performance the problem

In the final step, the data are acquired assessed in terms of the basic performance parameters; such as short-circuit current, open-circuit voltage, efficiency and maximum power output. In order to analyse and separate the effects, the spectral data used as illumination sources are also separated in terms of their average photon energy and broadband irradiance. The comparison between the illumination state, the state of the device and its performance characteristics enables to investigate and analyse systematic effects.
Chapter 2 – Optical Modelling

2.1. Introduction

Optimization of light management in hydrogenated amorphous silicon (a-Si:H) solar cells has already been understood well enough to provide significant advances in the efficiency of a-Si:H PV devices. As a result, it has been realised that understanding and furthermore improving a-Si:H solar cells cannot be achieved without an understanding of their underlying optical behaviour.

Reduction of the absorption of the front electrically inactive layers such as the glass and the TCO [26] and enhancement of the light confinement within the absorber layers have been both recognised as crucial to achieve high efficiencies [26] for all thin-film silicon solar cells. An overview of the different mechanisms leading to optical losses in a-Si:H solar cells is displayed in Figure 9. As light confronts the top surface of a solar cell, photons are subjective to:

![Diagram of a-Si solar cell with rough interfaces and mechanisms of optical losses](image)

**Figure 9:** Schematic cross section of a typical a-Si solar cell with rough interfaces. The arrows represent incoming, reflected, transmitted and scattered light. The major mechanisms of optical losses and the concept of light confinement are visualised.
i) reflection at the top glass-air interface, which can be primary, secondary or a product of multiple internal reflections,

ii) early absorption by the front electrically inactive layers, such as the glass and TCO

iii) delayed absorption by the back electrically inactive layers, such as buffer layers and the back contact.

The reason for ii) and iii) is the nature of the absorption of the materials used in thin-film silicon devices. Whereas absorption is high for short wavelength light, it strongly decreases towards longer wavelengths as the light energy approaches the band gap of a-Si:H. Therefore, very short wavelengths (λ<380nm) are almost fully absorbed by the front inactive layers, while longer wavelengths (λ>480nm) inevitably suffer from incomplete absorption. This increases progressively with increasing wavelength. The total absorption decays to close to zero for wavelengths in the range of a-Si band gap\(^1\) (λ≈800nm). Hence, the photovoltaic effect in amorphous silicon solar cells may be limited between the TCO cut-off region and a-Si:H band-gap, but its effectively reduced further by incomplete absorption.

This is demonstrated in Figure 10, where the variation of the wavelength dependent light absorption\(^2\) is examined for three different materials used in a-Si:H solar cells; glass, TCO (ZnO) and a-Si:H bulk and two different optical depths. The thinnest and thickest thickness encountered in modern a-Si:H solar cells [27] is also indicated. In this simplified examination multiple reflections were not taken into account and light absorption was assumed to decay exponentially as defined by Beer–Lambert–Bouguer\(^3\) law. Strictly speaking, thickness here does not represent the physical thickness of a layer, but the optical path. The graph though, indicates characteristically the wavelength

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\(^1\) It is established in literature that the gap of a-Si is 1.72eV (≈721nm) eg. [28]. Bruns et al. [29], have shown a-Si:H solar cells with responsivity well above the band gap, which often reach values as high as 1.55eV (≈800nm). Kopidakis has shown the influence of meta-stable defects and band-tails in a-Si:H optical absorption, which essentially extend its range even up to 1.51eV (≈820nm). In this work a-Si bandgap refers to the responsivity edge of a-Si:H with typical defect density \(10^{15}\)-\(10^{16}\), which is approximated at 1.55eV (≈800nm) [28].

\(^2\) Typical absorption coefficients used in a-Si:H PV technologies were utilised, such as given by Springer et al. [31].

\(^3\) The law states that there is a logarithmic dependence between the transmission (or transmissivity), T, of light through a substance and the product of the absorption coefficient of the substance, \(a\), and the distance the light travels through the material (i.e. the path length), \(\ell\).
window, where the photovoltaic effect occurs in amorphous silicon technologies, as well as the range where incomplete absorption takes place.

![Wavelength dependence of light percent absorption for different materials used in a-Si:H solar cells; glass, TCO (ZnO) and bulk a-Si:H. The notation next to each materials represents the optical depths assumed in each case.](image)

Figure 10: Wavelength dependence of light percent absorption for different materials used in a-Si:H solar cells; glass, TCO (ZnO) and bulk a-Si:H. The notation next to each materials represents the optical depths assumed in each case.

Particular interest in current developments is on methods which eliminate optical losses and confine the light within the a-Si absorber. These methods are encountered in literature with different names such as “light management schemes” (LMS) or “light confinement strategies” (LCS) or simply as “light trapping”. Early attention [32] has been given to the employment of total internal reflection (TIR) by the use of a progressively increasing grading of the refractive index from glass to the a-Si:H absorber and the layers in between. Incident photons which arrive at an interface with an angle larger than the critical angle towards the front electrode are “trapped” within the structure and therefore, the total reflection at the top of the cell is reduced. Nowadays, sophisticated methods, which are still based on the principle of TIR, are used in a-Si:H solar cell technologies. For instance Krč et al. [33] have shown optimised light confinement by the use of nano-size reflecting interlayers, while Peters et al. [34] have exploited photonic crystals, which can act as angularly selective filters to
maximise light trapping at a wavelength region of 650-750nm and therefore, reduce reflection at the top of the cell.

For amorphous or microcrystalline thin film silicon solar cells light trapping is also achieved by nano-texturing substrates, which introduce rough interfaces in the solar cell and take advantage of light scattering. Specifically, by pyramidal texturing of the front surface of the solar cell [35] multiple reflections occur at the front surface, which reduce reflection losses. The average photon path length is also increased by changing the direction of the light in the solar cell by refraction. Typically, the light trapping structure is combined with an anti-reflective coating to further decrease front surface reflection losses [36]. The optical path length enhancement for this technique is in the range of a factor of $\ell=10$ [34]. However, current solar cells, which become thinner and thinner, require more efficient light trapping mechanisms. A commonly used method is scattering of light inside thin-film solar cell. Part of the light which reaches nano-rough interfaces is scattered in various directions instead of propagating in the specular direction [38], as shown in Figure 9. Hence, the average photon path is further extended. Combining scattering with total internal reflection, a theoretical path length enhancement of an empirical factor $\ell=4n^2$ [34],[37] is achieved, with $n$ being the refractive index of the material.

![Incomplete absorption bandwidth](image)

Figure 11: Absorption potential (%) of a 250nm a-Si:H mono-layer as a function wavelength for three cases of optical depth $\ell$: i) $\ell=250$ nm ii) $\ell=10\cdot250$ nm and iii) $\ell=4n^2\cdot250$ nm. The bandwidth of the incomplete absorption is noted on top.
This is displayed in Figure 11 where the absorption potential of a typical 250 nm a-Si:H mono-layer was examined assuming an optical depth (i) $\ell=250$ nm, (ii) $\ell=10\cdot250$ nm and (iii) $\ell=4n^2\cdot250$ nm, where $n$ is the refractive index of a-Si:H. It is shown that increasing the path length via light management schemes, such as TIR and scattering mechanisms is crucial for reducing incomplete absorption and optimising the optical absorption. Despite the optical path being based on simplistic and empirical approaches, the graph above retains a realistic similarity with published experimental measurements eg. [39]. In any case the method does not contain sufficient information to holistically characterise the optical performance of a-Si:H solar cells, and should only be treated as a first order approximation. An overview of the optical models, which have been developed to optically analyse a-Si:H solar cells, is the subject of the discussion carried in the following section.

### 2.2. Overview of Optical Modelling in a-Si:H Solar Cells

Optical modelling is an important tool for the analysis of loss mechanisms, and the optical enhancement of a-Si:H solar cells. Experimental methods to estimate light absorption profiles and quantify optical losses within amorphous silicon thin-film devices have been suggested, but are difficult to implement and are subjective to experimental difficulties (e.g. Hohne et al. [40]). On the other side optical modelling enables a relatively easy and inexpensive quantitative comparison of optical performance of alternative materials. It allows the optimisation of the physical structure of the device and its underlying loss mechanisms. Furthermore, it allows direct access the calculation of electron-hole pair generation profiles within the absorber. For this reason optical modelling has gained significant momentum, as a method to optically characterise thin-film solar cells.
Due to this extensive literature grown in the field of optical modelling of thin-film solar cells, it is indeed a difficult task for one to mention all the models, which have been published so far. Thus, in this section we will only focus on the most significant modelling milestones with particular interest to recent literature, which is dedicated to the simulation of a-Si:H solar cells. Scientists, such as Rowlands et al. [41], suggest that a detailed optical simulation of these devices would include specular and scattered components of the light (Figure 12), simulation of the morphology of the interfaces, interference and geometrical features in a three dimensional universe. As a result the optical analysis of a-Si:H solar cells may often depend on input parameters, which are challenging to be experimentally measured, and it is computationally impeded by the difficulties solving rigorously the Maxwell equations (Haase et al. [42]). To overcome these difficulties, all models initiate simplifications, and hence the accuracy of every model is subjective to the degree of their accuracy.

Leblanc et al. [43] have proposed a semi-empirical, one-dimensional model for a-Si:H solar cells based on experimental observations for reflectance and assuming mean paths for the light propagation within every layer. Although in this model scattering of rough interfaces was taken into account only two interfaces were assumed to be rough: the TCO – p-layer and the n-layer – back reflector. Later Prentice [44] presented an one-dimensional analytical method to characterise optical absorption profiles in a-Si:H thin-film solar cells, based on an incoherent light interference. While this method is not computationally demanding and is independent of empirical approximations, it also does not take into account scattering effects. Tao et al. [45] have suggested a two dimensional semi-empirical approach. In this an interface acts as reflection and transmittance centre of varying solid angle distribution, where the TCO – p-layer and the n-layer – back reflector interfaces acted as scattering centres. Later Zeman et al. [38] extended the model by introducing scattering at all interfaces and carried a more thorough examination on the haziness$^1$ of the involved materials. This model makes a simplification to rigorously treat Maxwell equations. Firstly, the reflective and transmittance of each layer is determined within a single loop; effectively treating each layer as an interface. Therefore, it does not take into account the polarization of light,

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$^1$ The haze parameter, or haziness, of a material is the ratio between the scattered part of the reflected (transmitted) light to the total reflected (transmitted) light at a specific wavelength $\lambda_0$. 
nor the scattering of already scattered light encountering a rough interface. These models may seem outdated by today’s standards, but were fundamental and formed the basis for the development of models such as the ones discussed in the next paragraphs.

Krc et al. [26] have suggested a one dimensional model, which light is treated as propagating electromagnetic waves. This model assumes that all internal rough interfaces cause light scattering. The scattering properties of individual interfaces are described by statistical parameters such as haziness and angular functions. The innovation of this model is it takes into account interference of coherent non-scattered light. The only limitation in this model [46] is its limitation to one dimension. Therefore average photon paths for oblique angles are underestimated. It should be noted, however, that two dimensional corrections were taken into account for the scattered part of the light. A similar approach was followed by another group, Springer et al. [31], who also studied the optical absorption in a-Si:H solar cells. In this model light was also treated as an electromagnetic wave propagating in one dimension, which scatters at rough interfaces. In this approach the average photon path of the scattered light was estimated by Monte-Carlo simulations in a three dimensional space. These calculations did not include the specular part of the light.

Alternative models have also been suggested such as the one proposed by Haase et al. [42], who studied the effects of periodic structures in a-Si:H. The examination is based on a three dimensional optical analysis software, specialised to rigorously solve Maxwell equations. This model uses the finite integration technique (FIT)\(^1\), which solves the propagation of light within a finite elements grid, by applying the so-called Maxwell-grid equations. In this examination however, light is diffracted uniformly in each layer, which may not be the case, as other scientists have shown ([26], [31], [38]). Additionally, mesh density plays an important role in the finite integration schemes, and may act as a source of additional errors. Rowlands et al. [47] characterised the optical behaviour of a-Si:H solar cells using an effective medium approximation (EMA)\(^2\). This method is basically a one dimension model, which assumes that light interacts with the

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\(^1\) The finite integration technique (FIT) is a spatial discretisation scheme to solve electromagnetic field problems in time and frequency domain numerically. It preserves basic topological properties of the continuous equations such as conservation of charge and energy.

\(^2\) Effective Medium Approximations (EMA) are physical models that describe the macroscopic properties of a medium based on the properties and the relative fractions of its components. They all assume that the macroscopic system is homogeneous and typical of all mean field theories.
thin nano-rough layer, as if it is a distinct layer with intermediate optical properties. The model differentiates the effects of nano-roughness, that is roughness having in-plane correlation lengths smaller than the wavelength of light and macro-roughness, which is roughness having in-plane correlation lengths of the order of the wavelengths of interest. According to this theory, the second is responsible for scattering effects, while the first will cause a distortion in the classic treatment of absorbance and can be modelled using EMA. Nevertheless, this model does not take into account the effects of macro-roughness and also uses the linear symmetry theory, which is considered less accurate comparing to other EMA, such as Bruggelman’s approach [41].

Other methods, which are significantly less involved, have also been proposed for the simulation of a-Si:H solar cells, such as the ones by Hegedus et al. [25] and Krauter et al. [48]. These models may use crude approximations, such as ignoring scattering, or assuming the total reflectance, but demonstrated a reasonably good accuracy.

It is important to note that each of the above mentioned models makes approximations, and is impeded by them. However, there is no good or bad model, but every model has to be treated individually and reviewed on the basis of the effect, which is being designed to examine.

2.3. Optical model development

As briefly discussed in chapter 1 the primary subject of this thesis is not the study of structural details of a-Si:H solar cells, which is known to require a thorough optical examination ([26], [31], [38]), but the investigation of a-Si:H solar cells performance under varied indoor and outdoor spectra. Scientists such as Krauter [48] have already shown that examination of intensity variations of outdoor conditions is possible even with crude optical assumptions. However, spectral variations of indoor and outdoor spectral conditions require a more thorough examination, as often the examined spectra have very thin \( APE \)\(^1\) differences of less than 0.05eV. Hence, it is a matter of scientific methodology to follow an approach, which can accurately simulate the magnitude of the

\(^{1}\) The \( APE \) is the abbreviation of the Average Photon Energy of a spectrum.
examined effects. To do so, the approach followed in this work is based on the propagation of EM waves and is similar to the work of Krc [46], and Springer [49], but extended into a two dimensional space. In the following sections the main aspects of the model will be described.

2.3.1. Electromagnetic wave propagation and absorption in a homogenous medium

Figure 13: Electromagnetic waves can be imagined as a self-propagating transverse oscillating wave of electric and magnetic fields. This diagram shows a plane linearly polarized wave propagating from right to left. The electric field is in a vertical plane, the magnetic field in a horizontal plane [50].

For plane waves Maxwell's equations impose the transversality requirement that the electric and magnetic field be perpendicular to the direction of propagation and to each other [51]. The electromagnetic wave propagation in its most general form is given by the exponential expression (1), or its alternative trigonometric form (2):

\[
\vec{E}(\vec{k},t) = \text{Re}[\hat{0}, E_y, E_z \exp(j \cdot \phi)] \cdot \exp(j(k \cdot x - \omega \cdot t)) \\
\vec{E}(\vec{k},t) = (0, E_y \cos(k \cdot x - \omega \cdot t), E_z \cos(k \cdot x - \omega \cdot t + \phi))
\]

where \(E_y\) and \(E_z\) are the amplitudes of the \(y\) and \(z\) directions, \(\vec{k}\) is the direction of propagation, \(k \equiv 2\pi/\lambda\) is the wavenumber, \(\phi\) the phase difference, \(x\), the position towards the direction of propagation and the time is \(t\).

The complex refractive index \(\tilde{N}\) for a material is given as [51]:

\[
\tilde{N}(\lambda) = n(\lambda) - j \cdot \kappa(\lambda)
\]

Here \(n\) and \(\kappa\) are the real and imaginary components of the complex index of refraction.
The attenuation of the wave within a homogenous medium is given by Beer–Lambert–Bouguer Law [51], which is described mathematically as:

\[ I(x) = I_0 \exp(-\alpha \cdot \ell) \]  

(4)

where \( \ell \) is the path length on the direction of propagation \( \vec{k} \), and \( \alpha \) is the attenuation (or absorption) coefficient, related to the imaginary part of the complex refractive index, \( \kappa \), at wavelength \( \lambda \) with the expression [51]:

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

(5)

2.3.2. Polarisation and electromagnetic wave propagation of light within two media

By convention, the polarization of light is described by specifying the orientation of the wave's electric field at a point in space over one period of the oscillation. The electric field vector of a plane wave may be arbitrarily divided into two perpendicular components labelled \( \vec{E}_y \) and \( \vec{E}_z \), while \( x \) is the direction of the transverse wave propagation. These two components have always the same frequency, but may differ at their amplitudes \( |E_y| \), \( |E_z| \) and their phase \( \varphi \). Both amplitudes \( |E_y| \) and \( |E_z| \) of the electric field and the phase determine the state of polarisation, which can be linear (when \( \Delta \varphi = 0 \)), circular (when \( \Delta \varphi = \pi/2 \) or \( -\pi/2 \) and \( |E_y| = |E_z| \)), or elliptical (when \( \Delta \varphi \neq 0 \) and \( |E_y| \neq |E_z| \)). Solar radiation light is an electromagnetic wave composed by the superposition of wave trains of random polarisation. Such a wave is said to be unpolarised [51]. In practice most common light sources used in solar simulators such as incandescent and fluorescent light bulbs produce unpolarised light.
When light moves from a medium of a given refractive index $n_i$ into a second medium with refractive index $n_t$, both reflection and refraction may occur. While the angle of reflection, $\theta_r$, is the symmetrical projection of the angle of incidence, $\theta_i$, to the surface normal (Figure 14), the relationship between the angle of incidence and the angle of refraction, $\theta_t$, is determined by Snell’s law [51]:

$$n_i \sin \theta_i = n_t \sin \theta_t$$

(6)

The intensity variation of the reflected, $r_0$, and the transmitted, $t_0$, components, as well as their polarisation state, depend on the intensity of the incident light and its polarisation. The relationship is determined by Fresnel coefficients [51].

For the component of the electric field which is perpendicular to the plane of incidence:

$$r_{0\perp} \equiv \left( \frac{E_{0r}}{E_{0i}} \right)_{\perp} = \frac{n_i \cos \theta_i - n_t \cos \theta_t}{n_i \cos \theta_i + n_t \cos \theta_t}$$

(7)

$$t_{0\perp} \equiv \left( \frac{E_{0r}}{E_{0i}} \right)_{\perp} = \frac{2 n_i \cos \theta_i}{n_i \cos \theta_i + n_t \cos \theta_t}$$

(8)

While for the component of the electric field which is parallel to the plane of incidence:

$$r_{0\parallel} \equiv \left( \frac{E_{0r}}{E_{0i}} \right)_{\parallel} = \frac{n_i \cos \theta_i - n_t \cos \theta_t}{n_i \cos \theta_i + n_t \cos \theta_t}$$

(9)

$$t_{0\parallel} \equiv \left( \frac{E_{0r}}{E_{0i}} \right)_{\parallel} = \frac{2 n_i \cos \theta_i}{n_i \cos \theta_i + n_t \cos \theta_t}$$

(10)

The quantities $E_{0i}$, $E_{0r}$ and $E_{0t}$ are the amplitudes of incident, reflected and transmitted components of the electric field of the EM wave.
2.3.3. Light Intensity and electron-hole pair generation

The intensity $I_r$, or radiant flux density, is the time-averaging pointing vector $\vec{S}$, which is related to the vectors of the electric $\vec{E}$ and the magnetic field $\vec{B}$. For the case of a propagating sinusoidal electromagnetic plane wave of a fixed frequency the following equation holds:

$$I \equiv \langle \vec{S}(x) \rangle = \frac{c}{8\cdot\pi} \cdot \text{Re}[\vec{E}(x) \times \vec{B}^*(x)] \frac{4\cdot\pi\cdot k}{\lambda_0} \Rightarrow I = \frac{c\cdot\epsilon}{2} E_0^2$$  \hspace{1cm} (11)

Equation (11) is simplified, since the time, or space average of $\cos^2(k \cdot r - \omega \cdot t)$ is $\frac{1}{2}$. The superscript * indicates a conjugated complex number and $c$ represents the velocity of light in vacuum. The quantity $\epsilon$ is called permittivity and is related to the refractive index and permeability by the relationship:

$$n = \sqrt{\epsilon \cdot \mu}$$  \hspace{1cm} (12)

For most materials, $\mu$ is very close to 1 at optical frequencies.

When a photon interacts with amorphous silicon and photon energy is higher than a-Si:H band-gap, an electron-hole pair will be generated. The number of electron–hole pairs generated by one absorbed photon in a-Si:H can be assumed to be unity [38]. The charge carrier light-induced generation profile $G_L(x,\lambda)$ is then calculated by the following formula:

$$G_L(x,\lambda) = -\frac{\lambda}{\hbar \cdot c} \left| \frac{dI_m(x,\lambda)}{dx} \right|$$  \hspace{1cm} (13)

where $\hbar$ is Planck constant. To determine the total charge carrier generation, $G_L(x)$, of the whole spectrum, all the discrete wavelength contributions $G_L(x,\lambda_i)$ are summed up [46].

$$G_L(x,\lambda) = \sum_{i=1}^{\infty} G_L(x,\lambda_i)$$  \hspace{1cm} (14)

$N$, here, is the total number of wavelength bins in the discretised spectrum.
2.3.4. Effective media approximation on pyramidal texturing of the glass coating

The effective media approximation (EMA) is a concept which allows calculating dielectric constant for a composite medium with homogeneous mixture of components on the scale smaller than the wavelength of electromagnetic wave. This approach can be used to simulate the effects of pyramidal texturing (Figure 15), of glass coatings, as shown by Springer [49].

The concept of EMA is not new, since it was proposed by Brugemann in 1935 [52] and is available in English literature in numerous essays and books e.g. [53]. The EMA was proposed to simulate the physics of interfaces separating two dielectric media. According to this theory, the rough interface is divided into M virtual layers, as shown in Figure 16. Every layer is regarded as an array of two components A and B. Optical properties of the layers are described by weighted refractive indexes, as well as the structure of the interface.

Specifically, every virtual interlayer is a mixture of both media A, B and its refractive index, $N_{EMA_i}$, is given by the formula:
\[ N_{EMA_i} = (1 - \gamma_i) N_A + \gamma_i \cdot N_B, \quad \text{where} \quad 0 < \gamma_i < \ldots < \gamma_M < 1 \]  

(15)

where \( N_A \) and \( N_B \) are the refractive indices of media A and B, and M the number of the virtual layers. The quantity \( \gamma_i \) represents the distribution of the variation and is dependent on the structure of the interface.

It is a matter of geometry to show that distributions, which correspond to pyramidically structured coatings, can be approximated by the following formula:

\[ \gamma_{pyramid}^i = 1 - \left( \frac{M + 1 - i}{M + 1} \right)^2 \]  

(16)

Knowing the refractive index of each virtual layer and assuming each layer has dimensionless thickness and hence no absorption, one can calculate the distribution of light within the virtual layers, as defined by Fresnel equations and Snell’s law. Simulations had shown that increasing the number of virtual layers to values higher than five did not have a significant effect on Absorbance-Transmittance-Reflectance (ATR) of the simulated structures. Figure 17 shows the difference in terms of ATR for a structure of 1mm glass monolayer with and without EMA of five virtual layers of pyramidal structure. It is shown that reflectance is being reduced for the interface with the pyramidal structure. In practice etching is applied at the TCO/Glass interface and pyramidal structures occur to reduce reflectance [26]. In such case EMA is a fair approximation [49].

Figure 17, a, b: Simulated ATR for 1mm glass monolayer assuming a planar interface (a) and with pyramidically textured coating (b) simulated by EMA of five virtual layers. The dotted lines correspond to the same y-axis height and are used to visualise the difference.
2.3.5. Light scattering at nano-rough interfaces

As a bundle of light bounces on a nano-rough interface, a part of the specularly reflected and transmitted components scatters to a random direction. As shown in Figure 12, for main components can be identified; specularly reflected, specularly transmitted, scattered reflected and scattered transmitted. This effect is well-known in literature and has been the studied by many independent scientists. First Beckmann and Spizzichino in 1963 studied the scattering of electromagnetic waves from rough surfaces and suggested the scalar scattering theory [54]. This theory was adopted and used for the optical simulation of a-Si:H solar cells with rough interfaces in many studies, such as Green [37], Krč [26], Springer [31] and Zeman [38].

The scalar scattering theory describes these losses by reducing Fresnel coefficients. The actual Fresnel coefficients are the product of the scattering factors, given by scalar scattering theory, and Fresnel coefficients [49].

\[ r_\perp = r_0 \perp \cdot s_r \quad \text{and} \quad t_\perp = t_0 \perp \cdot s_t \] (17)

\[ r_\parallel = r_0 \parallel \cdot s_r \quad \text{and} \quad t_\parallel = t_0 \parallel \cdot s_t \] (18)

Where the scattering factors \( s_r \) and \( s_t \), are defined by the equations:

\[ s_r = \exp \left[ - \frac{1}{2} \left( \frac{4\pi \cdot n_0 \cdot \sigma_{rms} \cos \theta_i}{\lambda} \right)^2 \right] \] (19)

\[ s_t = \exp \left[ - \frac{1}{2} \left( \frac{2\pi \cdot (n_i - n_0) \cdot \sigma_{rms} \cdot \cos \theta_i}{\lambda} \right)^2 \right] \] (20)

\( \sigma_{rms} \), often also denoted as \( r_{rms} \), stands for root mean square interface roughness between the layers.

Equations (19), (20) describe only the effect of scattering in terms of intensity of non-scattered light. The angular dependence of the scattered light is described by the angular distribution function (ADF), which relates the intensity and the scattering angle of every beam, as:

\[ I(\theta) = ADF(\theta) \cdot I_{arb} \] (21)

The quantity \( I_{arb} \) represents an arbitrary intensity.
Table III: Angular distribution functions of scattered light (ADF) used in this work

<table>
<thead>
<tr>
<th>Interface</th>
<th>ADF</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air / Glass</td>
<td>$\cos^2(\theta)$</td>
</tr>
<tr>
<td>Glass / TCO</td>
<td>$\cos^6(\theta)$</td>
</tr>
<tr>
<td>TCO / a-Si:H</td>
<td>$\cos^2(\theta)$</td>
</tr>
<tr>
<td>a-Si:H / Back Reflector</td>
<td>$\cos^6(\theta)$</td>
</tr>
</tbody>
</table>

For a perfect Lambertian surface (ideal diffusive surface), the intensity of light scattered in any given direction from this surface is proportional to the cosine of the angle between this direction and the direction normal to the surface, as shown in Figure 18, b [55]. However, not all interfaces respond like perfect Lambertian diffusers, experimental measurements ([46],[49]) had shown deviations, such as the amorphous silicon / back reflector interface (a-Si:H / ZnO:Ag), as shown in Figure 18, a. The angular distribution functions of interfaces involving in a-Si:H solar cells used in this work are based on empirical approximations of measurements published by Krč [46] and Springer [49] and are listed in Table III. One should note that in any case the simulated approximations of ADF do not differ significantly from their measurements (Figure 18, a and b).

Knowing the intensity and angular distributions of scattered light, the vectors of the electric field can be calculated for every scattered beam, based on the principle of energy conservation. In other words the energy carried by the reflected (transmitted beam) as given by the original Fresnel equations, should equal the energy carried by the
sum of reduced reflected (transmitted) and scattered reflected (transmitted) light. Since, the information is calculated individually for the perpendicular and parallel components of light, the information for scattered light has to be carried out again individually.

Hence, for the case of perpendicular and parallel components of reflected and transmitted non-scattered light the following equations hold:

\[ E_{r,\perp} = r_{\perp} \cdot E_{0,\perp} \quad \text{and} \quad E_{r,\parallel} = t_{\parallel} \cdot E_{0,\parallel} \]  \quad (22)
\[ E_{t,\perp} = r_{\perp} \cdot E_{0,\perp} \quad \text{and} \quad E_{t,\parallel} = t_{\parallel} \cdot E_{0,\parallel} \]  \quad (23)

Assuming the total radiant photon flux (~\(n \cdot \cos \theta \cdot E^2\)), which passes through the normal to the plane, does not change whether light scatters on not, the amplitude of the electric field for the total scattered light is:

\[ E_{sc,r,\text{tot},\perp} = \sqrt{E_{r,0,\perp}^2 - E_{r,\perp}^2} \quad \text{and} \quad E_{sc,r,\text{tot},\parallel} = \sqrt{E_{r,0,\parallel}^2 - E_{r,\parallel}^2} \]  \quad (24)
\[ E_{sc,t,\text{tot},\perp} = \sqrt{E_{t,0,\perp}^2 - E_{t,\perp}^2} \quad \text{and} \quad E_{sc,t,\text{tot},\parallel} = \sqrt{E_{t,0,\parallel}^2 - E_{t,\parallel}^2} \]  \quad (25)

Furthermore, since the ADF of scattered light is known (16) and the total energy must be preserved, the amplitudes of electric field of scattered light for every different scattered angle are given by the following expressions:

\[ (E_{sc,r}(\theta_{\text{sc,i}}))_{\perp,\parallel} = (E_{sc,r,\text{tot}})_{\perp,\parallel} \cdot \sqrt{\frac{\cos(\theta_{\text{inc}}) \cdot \text{ADF} (\theta_{\text{inc}})}{\sum_{\theta_{\text{sc,i}}=-\pi/2}^{\pi/2} \cos(\theta_{\text{sc,i}}) \cdot \text{ADF} (\theta_{\text{sc,i}})}} \]  \quad (26)
\[ (E_{sc,t}(\theta_{\text{sc,i}}))_{\perp,\parallel} = (E_{sc,t,\text{tot}})_{\perp,\parallel} \cdot \sqrt{\frac{\cos(\theta_{\text{i}}) \cdot \text{ADF} (\theta_{\text{i}})}{\sum_{\theta_{\text{sc,i}}=-\pi/2}^{\pi/2} \cos(\theta_{\text{sc,i}}) \cdot \text{ADF} (\theta_{\text{sc,i}})}} \]  \quad (27)

Where the angle of a scattered beam, \(\theta_{\text{sc,i}}\), receives values between \(-\pi/2\) and \(\pi/2\). For the purpose of the optical simulations forty independent scattered directions were assumed. Increasing the number further does not change significantly the optical profiles from 380 to 750nm; the required computational power however will dramatically increase. This is shown in Figure 19, for a representative case of monochromatic incident light of 450nm bouncing on a a-Si:H solar cell structure of 1mm Glass/500nm ZnO TCO layer/7nm \(\mu\)c-Si p-layer/400nm a-Si:H i-layer/10nm \(\mu\)c-Si n-layer/400nm: ZnOAg buffer layer-back reflector. The corresponding average roughness of all interfaces is 10nm with the exception of the n-layer – back refleector interface where an average roughness of 50nm.
was used. It is displayed that increasing the number of scattered beams up to 20 per reflection, or transmission, has a significant effect on the normalised generation rate. However, further increase of the scattered beams does not cause a momentous change.

Figure 19: Effect of the number of scattered beams per reflection, or transmission to the normalised generation rate. The two examples here correspond to monochromatic light of 550nm (a) and 650nm (b). It should be noted that the same number of beams will also occur for both reflection and transmission, so essentially the total number of beams is doubled.

Figure 20 demonstrates scalar scattering theory on air/a-Si:H/air 300nm monolayer structure. Figure 20, a displays the ATR assuming perfectly planar interfaces. Hence no scattering effects were taken into account. In Figure 20, b a root mean square roughness of 30nm at both interfaces was assumed. As a result, light scatters and the average photon path is prolonged, causing visible decrease at the transmittance of long wavelengths (λ>650nm).

Figure 20, a, b: Simulated ATR for a 300nm a-Si:H monolayer assuming a plane (a) and nanorough, \(r_{\text{rms}}=30\text{nm}\), (b) for wavelength bins from 380 to 750nm. The dashed lines are used as guidelines to visualise the differences.
2.3.6. Modelling Procedure

Figure 21: Sketch of the ray-tracing iteration scheme employed. Light distributes within a multi-layer structure and separates into reflected, transmitted and scattered components.

The calculation is carried out for every discrete wavelength, $\lambda$, of the incident spectrum. The main calculation procedure is an iterative ray tracing. Every beam is traced individually within the space of the structure, as well as the multiple beams, which generates when it encounters a boundary. The characteristics of every beam are then stored in a matrix, $M$. Specifically, their $x$ and $y$ position, the amplitude of the perpendicular and parallel vectors of the electric field, $E_{\perp}$ and $E_{\parallel}$, their phase, $\varphi_1$ and $\varphi_2$, and the angle of propagation ($0\pi-2\pi$). In the next step the intensity of beams is checked one by one against an intensity level, which triggers the stopping criteria separating the beams that will be treated in the next iterative circle and the beams that will be rejected. The iteration carries on till the beams travel within all layers of the structure and their individual intensity is less than the manually set trigger level, while the matrix $M$ is updated in every iterative circle. A schematic of this basic iterative process is shown in Figure 21.
Initially, the user defines structural parameters of the device. Specifically, the layers, their dimensions, root mean square interfacial roughness, $r_{rms}$, the complex refractive index, $N$, and the angular distribution function, $ADF$, at each interface. In the second step, the spectral data are defined; such as the number of starting beams and their position on the first interface, the spectrum and its intensity, the polarisation bias of the light and the phase of the electric field components. At this point the ray tracing procedure is initiated, as described above. It should be noted though, that in every iterative circle, the model records the beams, which propagate within electrically active layers as previously defined by the user. The specifics of the selected beams are recorded on a separate matrix, $G$, updated in every iteration. When the ray tracing process is over, the generation profiles are calculated.

Figure 22: Holistic flow chart demonstrating the algorithm of the optical model.

The ray tracing scheme may be the most computationally demanding part of the modelling procedure, but it is only a step in the whole modelling process. An overview of the algorithm employed in the optical model is shown in Figure 22.
In order to do so, the user has to select whether the light is partially coherent, or not. For coherent collinear beams, the programme calculates their interference characteristics separately. In the next step the time averaging Poynting vectors for interfering and non-interfering beams are calculated. In the end the generation profiles and the light distribution within the multilayer structure are evaluated.

Figure 23: Distribution of light absorption in different layers of a-Si:H p-i-n solar cells, for a cell of 600nm i-layer thickness (a). Generation rates for the 600nm i-layer cell within the i-layer, as excited by AM1.5G standard terrestrial radiation [56] (b).

An example of the results can be seen in Figure 23, a and b, where a typical a-Si:H solar cell multilayer structure was optically analysed. The simulated multilayer structure consists of 1mm Glass/500nm ZnO TCO layer/7nm µc-Si p-layer/a-Si:H i-layer/10nm µc-Si n-layer/400nm: ZnO-Ag buffer layer-back reflector. For this simulation pyramidal EMA of five layers was assumed at Glass/TCO interface. The ADF used are listed in Table III. The distribution of light absorption within layers is shown in Figure 23, a. This figure represents the optical quantum efficiency (OQE) of the device, which is a measure for the probability of a photon being absorbed [38]. The generation profiles are also shown (Figure 23, b), as a function of i-layer depth and wavelength, excited by standard terrestrial AM1.5G radiation.

Since the electrical model is one dimensional, the calculated generation profiles are reduced to one dimension (Figure 23, b). Therefore, in order to process an arbitrary photon flux of $A$ [Photons/cm$^3$/nm], one would arrive at the same result either by processing $N$ beams of photon flux $A/N$ [Photons/cm$^3$/nm], or one beam of photon flux $A$; providing, of course, the generation profiles are reduced to one dimension and the volume of the studied structure is the same for both cases. The result may be the same, but the computational requirements in the first case are increased by a factor of $N$. The difference is significant, considering at longer wavelengths ($\lambda$>650nm), tens of millions of beams for a single wavelength bin will have to be processed even with a single
starting beam. For this reason, the starting matrix, $M$, is reduced to the bare minimum of one initial beam. This issue, however, is also linked with the level of the intensity tolerance and will be discussed in the following section.

2.3.7. Robustness and Numerical Errors

The aim of this part of the work is to design an optical platform, which would be able to probe a-Si:H PV performance under varied indoors and outdoors conditions. In terms of optical modelling, this is viewed as differences at the generation profiles caused in the electrically active layers of the a-Si:H solar cell. However, such quantities are experimentally not observable directly, nor the distribution of light within a multilayer is. The typical experimental method, which is employed to obtain optical information on the absorption, reflection and transmission of light through a material is ATR spectroscopy. In this case, however, ATR spectroscopy does not offer significant information, since transmission in a-Si:H solar cells is in most cases, with the exception of bifacial cells, zero. Even knowing the reflection of a cell, this does not mean evaluation of the absorption within different layers is experimentally measurable. Alternative methods have been suggested, such as Höhne et al. [40], Nonomura et al. [57], based on Photothermal Deflection Spectroscopy (PDS), which require expensive hardware and are susceptible to errors [40]. Hence, it is not remarkable why optical models, which are designed to simulate a-Si:H thin film multi-layer structure (e.g. [26], [31], [38], [43]), validate the optical model through a comparison with the electrical characteristics of the cell, namely the $J-V$ or $EQE$. This will be done in this case as well, and is being the subject of discussion in chapter 3, section 3.

The practical difficulties, which hinder the optical validation through strictly optical means, do not prevent the understanding of the limitations of the model. Specifically, a number of limitations can be seen through theoretical calculations. Firstly, the model is capable of processing spectra with minimal spectral differences, as much as $\Delta \lambda = 1 \text{nm}$, and quantifying the result in terms of generation profiles, as shown in Figure 24. The examination is based on optical profiles for different materials used in a-Si:H solar cells, as given by Springer et al. [31].
The resolution of the tabulated spectrum of the optical data is 2nm. Therefore, for evaluating the values of the complex refractive index in between an approximation should be made. The estimation of the optical data in between of the measurements is based on cubic Hermite interpolation, which is a source of errors. The model’s ability to distinguish between wavelengths in terms of average photon wavelength is $\Delta \lambda = 1$nm ($\sim 0.008$eV for 380nm, $\sim 0.004$eV for 550nm and $\sim 0.002$eV for 750nm). In this work, the magnitude of the spectral variations is 0.2eV for indoor and 0.12eV for outdoor spectra, while the minimum spectral differences examined between two spectra are in the range of 0.05-0.01eV, which is at all cases higher than the model’s distinctive ability.

Therefore, the examination is valid, because it is prohibited to spectral differences with $\Delta \lambda \geq 1$nm.

Another crucial factor is the ability of the model to treat the incoming light without rejecting a significant part of the radiant photon flux. As previously referred, beams with “insufficient” energy are rejected based on a manually set trigger level for the radiant photon flux. In Physics, however, the total energy is preserved within a multilayer structure of $N$ layers. This can also be summarised as the sum of the total absorbance within the $N$ layers, the total reflectance and the total transmittance of the structure is unity.

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1. In the mathematical field of numerical analysis a cubic Hermite spline is a third-degree spline with each polynomial of the spline in Hermite form. The Hermite form consists of two control points and two control tangents for each polynomial [58].
The quantity $A_i$ represents the absorbance of each layer in the multilayer structure. Rejecting beams introduces a small error with respect to the fact that the theoretical sum will never be equal to one. However, this allows a direct estimation of the errors for each discrete wavelength, $\lambda$. The quantity $I_0$ represents the starting intensity of the first beam. The ATR characteristics of the same structure under two different levels of intensity tolerance, $10^{-8} \cdot I_0$ and $10^{-9} \cdot I_0$ respectively, are examined in Figure 25, a and b. A dashed line is used to indicate that decreasing the error tolerance has a noticeable impact on longer wavelengths, which evade full absorption. It is shown that intensity tolerance has a significant effect on longer wavelengths ($\lambda > 650$nm), where incomplete absorption is significant and the amount of rejected radiant flux is not negligible. It is also shown for the case of $10^{-9} \cdot I_0$ tolerance, that the error is negligible at the largest part of the spectrum (380-650nm), where errors do not exceed 0.1% at most, and is low in the spectral region between 650-700nm (errors vary between 1-3%). However, the error for wavelengths higher than 730nm may be significant and reach 15% at 750nm. Nevertheless, contribution of current for wavelengths higher than 720nm for AM1.5G spectrum does not exceed the 3.5% of the total collection of current minimising the impact of any arising errors considerably.

![Figure 25: Uncorrected ATR profiles of the same structure for two different intensity tolerance levels, $10^{-8} \cdot I_0$ (a) and $10^{-9} \cdot I_0$ (b). The guidelines indicate that decreasing the error tolerance has a noticeable impact on longer wavelengths.](image)

In Figure 26 the number of iterations and the number of processed beams per iteration circle is plotted against different wavelengths for two different intensity tolerances $10^{-8}$...
and $10^{-9}$. For every case the starting beam was one. It is shown that longer wavelengths ($\lambda>650\text{nm}$) require more iteration circles and generate a significantly higher number of independent rays, and therefore the computational demands are also higher. It is also shown that there is no linear relationship between the number of processed rays and the change of the intensity tolerance. A further decrease of the intensity tolerance by a factor of 10, generates tens of millions of beams per circle and may often prove unsupportable demanding for most desktop computers (especially for the case of longer wavelengths). An indicating calculation for 10,000,000 independent beams with a characteristic matrix of 8 elements each, for 100 iterations stored in double precision, would require 6.4GB of RAM. Therefore, in this examination the intensity tolerance is limited to $10^{-9}I_0$.

In order to reduce the error further and allow examinations of spectra extending to 750nm, an empirical approach was adapted. By monitoring the layer at which each independent ray triggered rejection, as well as its radiant flux, empirical factors which allowed corrections were calculated. The absorption of each layer and its underlying generation rates were modified accordingly to satisfy the principle of energy conservation. However, this approximation assumes that the energy of each rejected beam would be fully absorbed by this layer, and would cause a generation uniform with the uncorrected generation profile. Such corrections can be seen in Figure 23, a and b, where the graphs correspond to the corrected profiles. Their sum of ATR characteristics is unity.

![Figure 26](image-url)

**Figure 26:** Example of number of rays processed in each iteration circle for two levels of intensity tolerance, $10^{-8}I_0$ (a) and $10^{-9}I_0$ (b).
2.4. Conclusions

Experimental methods to quantify optical losses within amorphous silicon thin-film devices have been suggested. They are difficult to implement and are subjective to experimental difficulties. For this reason it is common practice to use modelling to optically characterise the distribution of light within a-Si:H solar cells.

This chapter describes an optical model developed, which allows the study of any thin film multilayer structures with random interface roughness within a two-dimensional universe. The optical approach is essentially ray-tracing, since every beam of light is treated individually based on fundamental physics, such as Maxwell equations. This is not the case for most models, which often initiate simplifications to avoid the analytical solution of each individual beam. On the other hand, the accuracy of the examined model is subjective to its intensity tolerance, which defines the threshold level of the beams that are being rejected. Simulations have shown longer wavelengths to evade full absorption resulting in a large number of untreated beams. In this case the model assumes generation of untreated beams is qualitatively similar to the treated beams and initiates corrections to satisfy the principle of energy conservation. For the purpose of calculation of scattering, the work is based on scalar scattering theory, which is a semi-empirical approach. An additional drawback of this model is its limitation to two-dimensions. Considering that the lateral dimensions of realistic thin-film structures are much longer and especially the cell length, which in this case has been ignored, this approximation holds without loss in the generality of the solution.

The purpose of this model is primarily to examine the effects of spectral variation on a-Si:H solar cell performance. Since the solution of the model is based on analytical calculations; its distinctive ability depends on the precision of the input data. In this case the optical profiles of the materials are given with 2nm intervals with an uncertainty of ±1 nm. Therefore the model is restricted to probe spectra of average photon wavelength difference, $\Delta \lambda \geq 1$nm. A comparison against experimental measurements in the frame of a holistic opto-electric model is the subject of the discussion in chapter 3.
Chapter 3 – Electrical Modelling

3.1. Introduction

Electrical modelling is the standard method used to analyse the electrical collection of a-Si:H solar cells. Equivalent electrical circuit modelling is used either to avoid the use of experimentation and estimate the collection of the device with rather simplified methods, such as equivalent electrical circuit modelling, or to examine problems, which are not subjective to experimentation by the use of detailed semiconductor modelling. Modelling would allow the analysis of problems, that are not easily studied with experimental methods, such as the effects of spectral variation of the radiant flux and device degradation state on a-Si:H solar cell performance. Specifically, parameters which cannot be directly controlled in the experiment, i.e. as the bandwidth profile of the illumination spectra, or the structure and state of the device, can be set to a desired level through a modelling interface. Modelling also enhances the level of understanding of a-Si:H devices. A simulation produces a representation of the functioning of the system and allows the separation of the whole into individual physical quantities, which otherwise would not be subjective to experimental observation, but can be directly controlled or examined through modelling. An example of such quantities would be the charge carrier density, or the distribution of the electric field.

Understanding the electrical behaviour of a-Si:H solar cells must include the properties of p-i-n junctions as well as the specific recombination mechanism of a-Si, which is partially driven by dangling bond recombination. Differences between amorphous silicon solar cell devices and other solar cell technologies, such as e.g. crystalline silicon (c-Si) solar cells, will be summarised in the following paragraphs.

Most PV technologies are based on a p-n junction, where the driving force of the PV effect is minority carrier diffusion. In amorphous silicon however, the lifetime of the minority carriers in the heavily doped p-type and n-type regions is small\(^1\) and does not allow sufficient collection for a significant contribution to the overall current. Due to

\(^1\) Several independent groups of scientists such as Kopidakis et al. [30], Pfleiderer et al. [62], Hack et al. [63], have suggested the lifetime of minority carriers in the heavily doped p-type and n-type regions to be less than \(10^{-10}\) s. An approximation of free carrier lifetime within the i-layer is in the order of \(10^3\) s.
this short diffusion length, the photogenerated carriers would virtually all recombine in the doped a-Si:H layers before reaching the depletion region of the p-n junction. Therefore, a-Si:H solar cells are designed in p-i-n junction configuration in contrast with the standard p-n junction of a crystalline silicon cells.

As discussed in chapter 2 in p-i-n configuration the i-layer not only serves as an absorber, but also acts as a widened space charge region with an electric field extending across its borders. The presence of this electric field is responsible for electron-hole pair separation and the carrier collection at the device terminals [27]. The heavily doped p-type and n-type layers may not contribute significantly to minority carrier diffusion current, but are responsible for establishing a field within the i-layer and provide low loss ohmic contacts between the i-layer and the external electrodes. Therefore, the driving force of the photovoltaic effect in a-Si:H solar cells is drift occurring in the i-layer, which is built-up by the heavily doped p-type and n-type layers.

In addition the major mechanism of recombination in a-Si:H solar cells is dangling bond recombination in contrast with most solar cells, such as c-Si, that are mostly affected by band-to-band recombination. This is caused by the difference between crystalline and amorphous solids. The former present long range order in the position of the atoms in the lattice, while the latter exhibit only short range order in their atomic structure [30]. Comparing crystalline and amorphous silicon, both have atoms which are four-fold

\[\text{Drift is the directional movement of a charge carrier under the presence of an electric field.}\]
coordinated and the average bond lengths and bond angles in a-Si are the same. However, the atomic structure of amorphous silicon lacks any order in the arrangement of the second and further nearest neighbours. It has been shown that a random network with each atom to be four-fold coordinated, has very high internal stresses, which are relieved by the presence of three-fold coordinated atoms [64]. These three-fold coordinated atoms are the dominant defect centres in a-Si. It has been also proposed by Pantelides [65] that the floating bond, i.e. 5-fold coordinated atom is also an important defect in the material. The presence of these defect states causes significant recombination in a-Si:H severely decreasing carrier collection. This difficulty is overcome by passivating the dangling bonds with Hydrogen; the defect density in pure amorphous Si is in the range of $\sim 10^{21}$ cm$^{-3}$, while hydrogenated amorphous Si has a defect density of $\sim 10^{15}–10^{16}$ cm$^{-3}$ [27]. The bonding arrangements in c-Si, a-Si:H and the major defect and passivation states in a-Si:H are schematically shown in Figure 27. Although, the defect density of dangling bonds in a-Si:H is significantly reduced, dangling bond recombination [66] still remains a major recombination mechanism of a-Si:H solar cells together with direct (band-to-band) recombination [63] of electron-hole pairs.

A schematic overview of generation, collection and capture events in a-Si:H solar cells is displayed in Figure 28. Photons, which are absorbed in the p-layer or n-layer (Figure 28, I and VI) with energy higher than the band-gap, will generate extra electron-hole pairs. As a result the extra electrons, which are the minority carriers, will recombine and consequently the extra holes as well. Photons which are absorbed in the i-layer are under the influence of the electric field caused by the donor and acceptor ionised impurities of the n-type and p-type layers respectively (Figure 28, II). Under this influence holes are attracted towards the p-layer, while electrons are repelled towards the n-layer. Assuming both p-type and n-type layers are almost perfect conductors, the majority carrier injection is then converted to carrier collection at the terminals of the device almost without any significant losses (Figure 28, III). Nevertheless, the carriers are also susceptible to recombination, which may occur while the carriers travel across the i-layer. Such recombination mechanisms may be either direct recombination (Figure 28, IV), or dangling bond recombination (Figure 28, V). A more thorough examination of the above mentioned effects with respect to electrical modelling will be carried in the following paragraphs.
Figure 28: Schematic representation of generation, collection and capture events within an a-Si:H solar cell. Events I and VI corresponds to absorption of a photon by the p-layer, or the n-layer respectively, which leads to recombination. Event II corresponds to the absorption of a photon within the i-layer, which may lead to successful collection (event III), direct recombination (event IV), or dangling bond recombination (event V).

A crucial factor governing electrical performance of amorphous silicon solar cells is the i-layer thickness. The material properties of bulk amorphous silicon are known to be heavily affected by degradation after prolonged light soaking [24] or annealing due to high operating temperatures [67]. Scientists, such as Tanner et al. [68], or Vorasayan et al. [69] have shown a connection between i-layer thickness and levels of degradation; thicker devices may have higher initial efficiency, however do suffer greater efficiency degradation. The observed degradation is generally attributed to an increase of dangling bond density in the bulk of a-Si and is referred in literature as Staebler-Wronski Effect (SWE) [24]. As dangling bond recombination depends both on the density of dangling bonds and the average electron-hole path, thicker i-layer a-Si:H solar cells are prone to higher electrical losses due to recombination. Moreover, increased i-layer thicknesses will reduce the strength of the electric field within the i-layer, which is the driving force for e-h separation in a-Si:H solar cells, and weaken carrier collection. Nevertheless, increased i-layer thickness is beneficial for the optical behaviour of a-Si:H solar cells. Therefore, the thickness of the i-layer is a delicate trade off between optical and
3.2. Overview of Electrical Modelling in a-Si:H solar cells

Electrical modelling is a useful tool for the performance assessment of amorphous silicon solar cells. Not only it can quantify the results of optical modelling in terms of carrier collection, and evaluate optical losses, but it can also provide a basis to study the electrical loss mechanisms of solar cells, that cannot be evaluated experimentally. The electrical behaviour of amorphous silicon solar cells can be simulated either by equivalent circuit modelling, or by semiconductor modelling. Both have advantages and disadvantages, which will be discussed in the following paragraphs.

3.2.1. Equivalent Circuit Modelling

![Elementary equivalent circuit of a solar cell with incorporating series Rs and parallel Rp resistances under forward bias conditions.](image)

Equivalent circuit modelling is often the simplest and easiest approach to model a-Si:H solar cell behaviour. An equivalent circuit refers to the simplest form of a circuit that retains all of the electrical characteristics of the original (and more complex) circuit; in this case the a-Si:H solar cell. A typical equivalent circuit which is used to describe realistically the behaviour of solar cells is shown in Figure 29. The equivalent circuit
consists of a current source and a diode representing the dark characteristics of the solar cell containing the internal electric field, necessary for driving photoexcited carriers to the external circuit. The current source generates a photocurrent density, \( J_L \), corresponding to the photoexcitation of excess carriers by solar radiation, \( G \). The realistic behaviour of the cell is ensured under the presence of parasitic resistances; series \( R_S \) and parallel \( R_P \). The first takes into account electrical losses due to the parasitic series resistances such as the TCO and the back contact and the second allows for leakage current across the junction. The device is considered ideal, when the effects of parasitic resistances (\( R_S=0, R_P=\infty \)) are insignificant to the device current density-voltage (\( J-V \)) characteristics.

The non-ideal \( J-V \) characteristics of a typical solar cell device, which are commonly found in literature (e.g. [70-72]), are expressed as:

\[
J(V) = J_{\text{dark}}(V) + J_{\text{shunt}}(V) - J_L \Leftrightarrow J(V) = J_0 \cdot \left[ \exp \left( \frac{V - J \cdot R_S}{A \cdot V_t} \right) - 1 \right] + \left( \frac{V - J \cdot R_S}{R_p} \right) - J_L \tag{29}
\]

Here the first term \( J_{\text{dark}} \) of equation (29) represents the diode \( J-V \) characteristics, the second term \( J_{\text{shunt}} \) the parasitic current density due to leakage and \( J_L \) is the photocurrent source. \( J_0 \) is the current density flowing from the diode in dark conditions and under reverse bias, a term often called as “reverse saturation current density”. The terms \( V_t \) equation (30) is the thermal voltage, \( V_t=kT/q \), where \( k \) is the Boltzmann constant, \( T \) the absolute temperature and \( q \) the elementary electron charge. The ideality factor, \( A \), has a value depending on the dominant mechanism of junction transport receiving values between 1 and 2 (\( A=1 \) if the transport process is diffusion and \( A=2 \) is drift in the depletion region) [71]. Equation (31) is implicit and is commonly solved using iterative methods such as Newton-Raphson (e.g. Dormand et al. [73]).

Although it is generally accepted that equivalent circuits can describe and model the electrical properties of amorphous silicon solar cell technologies (e.g Merten [74], Kusian [75], Hegedus [76], Holley [77]), the derivation of expression (30) is based on assumptions, which hold for the idealised p-n junction, that cannot accurately describe amorphous silicon solar cell technologies. As previously discussed the later are based
on p-i-n configuration, whose behaviour differs from the ideal p-n configuration. The assumptions made are summarised here as follows:

1. The device is divided in two types of quasi-neutral regions. One, where the space-charge density is assumed zero throughout and another depletion region where the carrier concentrations are assumed so small that the only contributions to space-charge-density comes from the ionised dopants. This is known as the abrupt junction [78] or depletion approximation [70].

2. The injected minority carrier densities are small compared to the majority carrier densities. This approximation is often referred to as the low-injection approximation [70], [78].

3. The net current flow in a diode due drift and diffusion under no or moderate external bias, is small, while drift and diffusion take significantly higher values. [70] This is equivalent to the statement that the carrier densities at the boundaries are related to the electrostatic potential difference across the junction [78].

4. Neither generation nor recombination current exists in the depletion region. The electron and hole currents are constant throughout the depletion region [70], [78].

Figure 30, a: Space-charge density in a p-n junction assuming an abrupt junction (black solid line) and a graded junction (grey dotted line). Figure 30, b: Carrier distribution under forward bias in a p-n junction assuming low injection.

The first assumption essentially sharpens up the borders of the p-n junction, as illustrated schematically in Figure 30, a. The second and third assumptions are visualised in Figure 30, b, and practically allow to estimate the populations of electrons.
at holes at the borders of the junction under forward bias. The first three approximations are also true for amorphous silicon cells. It is known that the p-type and n-type regions of a-Si:H solar cells are heavily doped. Specifically, the density of ionised dopants in the heavily doped p$^+$ and n$^+$ regions is usually in the range of $10^{18}$ to $10^{19}$ cm$^{-3}$ [29], [79]. The large density of states leads to excessive recombination rates, which consequently shorten minority carrier lifetime significantly ($\sim10^{-10}$ s, [62], [63]. Therefore it is a fair assumption to use the first two approximations due to the large concentration of dopants and the almost negligible minority carrier injection. Statement three is also true providing the first two assumptions hold. It is known (e.g. Burgelman et al. [80]) that net current flow in a p-n junction under low bias conditions is very low, while drift and diffusion currents may rise up to six orders of magnitude higher. This essentially allows relating the minority carrier populations at the boundaries of the depletion region with the applied voltage across the junction [70].

In contrast with the three first approximations, which are valid for a-Si:H solar cells, the fourth assumption does not. The fourth statement assumes that no current is generated in the depletion region and the integral of recombination and generation current flow across the depletion region is effectively zero. This may be the case for solar cells, which are based on p-n junction configuration, where the width of the depletion region is negligible compared to the thicknesses of p-type and n-type layers. However, this is clearly not the case for p-i-n junctions, where a thick i-layer layered between p-type and n-type layer acting as the main absorber. As discussed in chapter 2, typical thicknesses of the i-layer vary between 0.2$\mu$m and 1$\mu$m, while the heavily doped p$^+$-type and n$^+$-type regions usually vary between 7-20nm each. The majority of photoexcitation occurs within the i-layer, whereas the recombination current flowing in this region is also strongly affected by the presence of high defect densities. Therefore, generation and recombination currents across the i-layer cannot be neglected, as in fact they are predominantly responsible for current flow within a a-Si:H solar cells.

For this reason Merten et al. [74] based on the suggestions of Hubin et al.[66], have suggested a modification of the one-diode model. In this semi-empirical approach, the single diode model is adapted to include a term which explicitly takes into account recombination losses within the i-layer. This is achieved by adding a parallel current density source, $J_{\text{rec}}$, to the photocurrent source, $J_L$, with opposing current flow direction,
as shown in Figure 31. The mathematical expression of the recombination current is given by the following expression:

\[
J_{\text{rec}}(J_L, V) = J_L \cdot \frac{d_i^2}{(\mu\tau)_{\text{eff}} [V_{\text{bi}} - (V - J \cdot R_s)]} \tag{32}
\]

The term \(d_i\) refers to the i-layer thickness of the device. The built-in potential, \(V_{\text{bi}}\) is the built-in potential of the device. The effective mobility-lifetime product, \((\mu\tau)_{\text{eff}}\) is given by the expression:

\[
(\mu\tau)_{\text{eff}} = J_L \cdot \frac{\mu_n^0 \tau_n^0 \mu_p^0 \tau_p^0}{\mu_n^0 \tau_n^0 + \mu_p^0 \tau_p^0} \tag{33}
\]

Where \(\tau_n^0\) and \(\tau_p^0\) are the capture times of the electrons and holes respectively by neutral dangling bonds within the i-layer.

Figure 31: The Merten equivalent circuit, which takes into account the losses due to recombination in the i-layer.

The expression (32) can be deduced assuming the electrical field is constant within the i-layer and strong enough to mask the effects of the diffusion of the carriers [81]. This assumption is expected to be valid only for small or negative external voltages, for cells with thin i-layer and low defect densities [74]. This is not the case for heavily doped p⁺-i-n⁺ a-Si:H solar cells. In fact significant diffusion currents near to the doped contact layers will be present due to high carrier concentration gradients [27], [63]. It should note though, that these approximations were correct for the devices investigated by Merten, since the study was restricted to cells with low electric field and doping densities. Additionally, the electric field is not constant, but varies strongly within the i-

---

¹ The built-in potential, \(V_{\text{bi}}\), in a semiconductor equals the potential across the depletion region in thermal equilibrium and equals to \(V_t \cdot \ln(N_a \cdot N_p/n_i^2)\) [78], where \(V_t\) is the thermal voltage, \(N_a\) and \(N_p\) the doping concentrations of the p-type and n-type layers respectively and \(n_i\) is the semiconductor intrinsic concentration.
layer [27], [29], [63]. Therefore, Merten’s model may be an improvement over the standard one-diode model, however its assumptions do not always hold for a-Si:H solar cells under forward bias and therefore it should be treated with caution and understanding of the conditions its being applied to.

Another shortcoming of equivalent circuit modelling is its inadequacy to probe the differences of chromatic spectral radiation. In the standard single diode model, photoexcitation is treated as a bulk quantity $J_L$, evaluated either by applying single-diode model parameter extraction methods such as Sites et al. [82], or Chan et al. [83] on experimental measurements, or by applying empirical crude optical approximations. The first requires experimentation, which is not easily implemented. The method is case by case sensitive; meaning for each illumination condition one should separately estimate the quantity $J_L$ experimentally. There is a practical implication, as one would have to carry on separate $J-V$ characteristics measurements for each illumination condition. Even if someone is determined to do so, the method is impeded by further problems. Indoor solar simulator spectra cannot fully represent the chaotic variation of outdoor spectra, while outdoor measurements inherit secondary effects arising from the variation of the angle of incidence or the temperature.

Figure 32: Differences in the normalised generation rate between an exponentially decaying function and optical modelling. Two cases are shown for excitation of wavelength, 550nm (a) and 650nm (b).

An alternative method would be to take into account the thickness of the front layers first order transmissions or reflections e.g. Hack et al. [63], Hegedus et al. [25], and Al Tarabsheh [28]. In such approximations the propagation of light is considered an exponentially decaying function. This assumption though, is not true. Figure 32 shows the difference in the normalised generation rate of an a-Si:H solar cell as calculated by
optical modelling [84], and a simplified exponential decaying function. In the first approach the generation profile is assumed to decay exponentially. In the second a solar cell structure is considered. It should be noted that here the generation rates are normalised to their maximum value to avoid any issues with calibration due to reflection, or transmission losses. It is shown that the nature of generation rate cannot be described accurately by the exponential law of Beer-Lambert-Bouguer law. The deviations become more noticeable as wavelength increases.

Consequently, even if equivalent circuit modelling is used, more detailed optical approaches will have to be implemented for the estimation of $J_L$. It is possible, however, to cause the same $J_L$ under short-circuit conditions with different generation profiles. The profiles though, having a different depth distribution, will also have different response to voltage. Such cases cannot be investigated by equivalent circuit modelling, which treats the photogeneration, $J_L$, as a bulk quantity.

An additional issue with equivalent circuit modelling is its inability to describe the $J-V$ characteristics of an a-Si:H solar cell under different illumination conditions with one set of data for the fundamental parameters, which determine the currents through the diode. The parameters that govern the underlying recombination mechanisms of a cell cannot always represent the performance of the same cell under different excitation profiles. Namely these parameters are the saturation current, $J_0$, the recombination current, $J_{rec}$, and the ideality factor, $A$.

The $J-V$ characteristics of a 400nm i-layer a-Si:H solar cell under AM1.5G radiation (Figure 33, curve 3) are being fitted to the Merten model (Figure 33, curve 4) showing an agreement. The simplest optical case that does not require optical modelling is the dark characteristic of a cell. Hence, it was used as a benchmark to study whether or not the two methods would still agree under different illumination conditions, but the same modelling parameters. This would essentially, isolate any side influences from photogeneration, $J_L$.

Figure 33 shows the two curves under dark conditions; curve (1) being the dark characteristics of the same cell and (2) representing the dark $J-V$ corresponding to the parameters extracted by Merten under AM1.5G illumination. Curves (1) and (2)
progressively depart with increasing voltage. Specifically, the parameter extraction of the Merten model overestimates the recombination occurring in dark conditions. This is not to surprise, as the modelled was fitted based on AM1.5G illumination, where the recombination due to the increase of free carrier populations is higher. The effect is escalated by increase of voltage, as the assumption of constant and strong electric field does not hold any more under increased forward bias as Merten et al. [74] pointed out. The latter shows the limitations of the model in conditions of different illumination and increased forward bias. In other words the estimation of parameters based on the Merten model under AM1.5G illumination cannot uniquely describe the behaviour of a-Si:H solar cells under different illumination conditions with one set of common parameters.

For all the reasons mentioned in the above paragraphs, the spectral response of a-Si:H solar cells in this work is not evaluated by using equivalent circuit modelling. Even so, the method is a useful tool for the purpose of estimating the parasitic resistances of the device. In this work a multi-parameter simplex fitting [85] based on the Merten model is used to evaluate the series resistance, $R_S$, and parallel resistance, $R_P$, of the device using its experimentally measured $J$-$V$ characteristics. For this purpose the analytical method of Chan et al. [83] was used to provide a first guess of the model parameters describing the simplified one-diode model.

![Figure 33, a: J-V characteristics under dark and light conditions.](image-url)
3.2.2. Semiconductor Modelling

Numerical modelling of semiconductor devices based on the carrier transport equations, namely continuity, current density and Poisson equations, which describe holistically the device without approximations was first suggested by Gummel [86] in 1964 for bipolar transistors. This approach was further developed and applied to p-n junctions by De Mari [87] and to IMPATT\(^1\) diodes by Scharfetter and Gummel [88] in 1969. Since this day the approach has been commonly used to model a variety of semiconductor applications and is usually referred to as the Gummel-Scharafetter method.

In photovoltaic technologies the method was adapted by Clugston et al. [89], who published “\texttt{PC1D}”, a simulation software with particular focus to c-Si and III-V compound materials, mainly GaAs and InP, solar cells. Burgelman et al. [80] published “\texttt{SCAPS}”, a numerical device simulator for thin film solar cells, which is mainly suitable for modelling polycrystalline thin film solar cells based on CdTe and CIGS technologies.

The solution of the carrier transport equations in a-Si:H solar cells was the field of research of several independent groups. Pfleiderer et al. [62] and Al Tarabsheh [28] have semi-analytical solutions, while their study was based on the assumption the electric field is constant throughout the i-layer. As previously discussed this is not always true for a-Si:H solar cells, especially under increased forward bias conditions. Hack et al. [63] and Chatterjee et al. [90] presented a full solution of carrier transport equations based on the Gummel-Scharafetter iteration method. However, in their approach the recombination term in the continuity equations is defined by Shockley-Read-Hall trap assisted recombination model, which is limited by minority carriers. In contrast dangling-bond recombination, is limited by majority carrier density [66]. A similar approach was followed by Wentick et al. [91], who also designed a detailed a-physical a-Si:H p-i-p device simulator, “\texttt{ASA}”. The work later was later further developed by Zeman et al. [92] to simulate a-Si:H solar cells and a-Si:H/a-Si:H tandem structures. Bruns et al. [29], studied the bias dependent spectral response of a-Si:H solar cells based on the same principles. It should be noted though, that all models are based on Gummel-Scharafetter method of solving the carrier transport equations. The

\(^{1}\) The IMPATT (Impact Ionization Avalanche Transit-Time) diode is a high power diode used in high-frequency electronics and microwave devices.
principles of this method, together with a synopsis of the underlying fundamental theory used will be the subject of the discussion in the following paragraphs.

3.3. Fundamental Theory Concepts

This section is a summary of the carrier transport equations namely, current density, continuity and Poisson equations, which govern the electrical behaviour of semiconductors. These equations carry no significant approximations, and can be derived from Maxwell’s equations. Therefore, they have a general effect, and can be considered fundamental.

3.3.1. Carrier Drift, Diffusion and Current Density Equations

The electrons in a semiconductor are moving rapidly and chaotically in all directions. Such movement is known as thermal motion. When a small electric field, \( \xi \), is applied to the semiconductor, each electron will experience a force \(-q \cdot \xi\) from the field and will be accelerated in the opposite direction of the field till it collides to lateral atoms, or other scattering centres. The transport of carriers under the influence of an applied electric field produces a current called the drift current. The electron current density, \( J_n \), flowing in a semiconductor is given by the expression [78]:

\[
J_n = q \cdot n \cdot \mu_n \cdot \xi
\]  

(34)

where \( \mu_n \) is the electron mobility, \( n \) the free electron concentration in the semiconductor and \(-q\) the elementary charge of an electron. Similarly for holes, which have a positive charge \(+q\), but move towards the opposite direction, the expression becomes:

\[
J_p = q \cdot p \cdot \mu_p \cdot \xi
\]  

(35)

where \( p \) is the hole concentration in the semiconductor.

Another important current component is the diffusion current. It exists when there is a carrier concentration gradient within the semiconductor material. In this case, the carriers move from a region of high concentration to a region of low concentration. For
electrons the diffusion current is proportional to the spatial derivative of the electron density [78], as given by the following expression:

\[ J_n = q \cdot D_n \frac{dn}{dx} \]  

(36)

\( D_n \) is the diffusion coefficient related to carrier mobility with the Einstein relation:

\[ D_n = \frac{kT}{q} \cdot \mu_n \]  

(37)

For holes, expressions (36) and (37) become:

\[ J_p = -q \cdot D_p \cdot \frac{dp}{dx} \]  

(38)

\[ D_p = \frac{kT}{q} \cdot \mu_p \]  

(39)

When an electric field is present together with a variation of carrier concentration, both drift and diffusion currents will occur. The current density equations for both electrons and holes are given in the following formulas:

\[ J_n = q \cdot \mu_n \cdot n \cdot \xi + q \cdot D_n \cdot \frac{dn}{dx} \]  

(40)

\[ J_p = q \cdot \mu_p \cdot p \cdot \xi - q \cdot D_p \cdot \frac{dp}{dx} \]  

(41)

while the total current flow in the device is given as the sum of electron and hole current densities, and should be constant across a device in equilibrium [78]:

\[ J = J_n + J_p \]  

(42)

Figure 34: Distribution of electron-hole concentrations within the i-layer of a-Si:H solar cell. In this case the cell was illuminated from the p-side (left), therefore the electron minority concentration (left) is significantly higher than the hole minority concentration (right).
A typical example of electron and hole distributions and current flows through a device is given in Figure 34 and Figure 35, where a 400nm i-layer a-Si:H solar cell is simulated under AM1.5G standard test condition radiation. In Figure 34 the electron-hole distributions of the device were simulated under short circuit and open circuit conditions. A strong asymmetry in the populations of electrons and holes is visible under low applied voltage conditions. This is due to the fact light enters through the p-layer of the device, and consequently increases the populations of the free carriers, which are located close the p-layer/i-layer interface. The effect is virtually negated, under increased applied bias conditions, where the increase of the free electron and hole population is substantial. In Figure 35, the corresponding current flows to the electron-hole distributions are computed. It is shown that although the individual drift and diffusion components of electron and hole currents may be significantly high, their summed quantities electron, $J_n$, and hole, $J_p$, current densities are much smaller, as already discussed in the third assumption of subsection 3.2.1. The total current flow is constant throughout the junction in equilibrium for any applied bias e.g. shown here for short circuit (Figure 35,a) and open circuit (Figure 35,b) conditions.

Figure 35: Current densities flowing through a p-i-n junction a-Si:H solar cell. The cell was illuminated from the p-side with AM1.5G radiation. The graph illustrates the current densities for short-circuit (a) and open-circuit (b) conditions.
3.3.2. Continuity Equation

The continuity equation describes the distribution of carriers in a semiconductor material where drift, diffusion, generation and recombination occur simultaneously. The continuity equation for electrons and holes expresses mathematically the conservation of the net carrier population flowing within an infinitesimal semiconductor element of thickness, $\delta x$ during a time change, $\delta t$. In other words the net current flow of ingoing and outgoing electrons or holes in a semiconductor slice should equal the net carrier recombination and generation occurring within the slice.

The incoming and outgoing carrier population is found by summing up algebraically the individual components and dividing the currents at each side of the slice by the charge of the electron. The nomenclature used for generation and recombination rates is $G$ and $R$ respectively, with $n$, or $p$ indicating the charge carrier is an electron or a hole respectively. Therefore the total rate of change for electrons is given by equation (43) [78].

$$\frac{\partial n}{\partial t} \cdot A \cdot dx = \left[ \frac{J_n(x)}{-q} - \frac{J_n(x + dx)}{-q} \right] \cdot A + \left[ G_n(x) - R_n(x) \right] \cdot A \cdot dx$$

(43)

where $A$, is the area of the slice. Expanding expression (43) into Taylor series yields to the time-dependent continuity equation for electrons (44) [78].

$$\frac{\partial n}{\partial t} = \frac{1}{q} \frac{\partial J_n}{\partial x} + G_n - R_n$$

(44)

Under equilibrium the carrier populations are time-independent; therefore equation (44) can be rewritten as:

$$- \frac{1}{q} \frac{dJ_n(x)}{dx} = G(x) - R(x)$$

(45)

Equation (45) is the time-independent continuity equation for electrons. A similar expression can be derived for holes, as shown below:

$$\frac{1}{q} \frac{dJ_p(x)}{dx} = G(x) - R(x)$$

(46)
Solving continuity equations for a known electrical potential distribution, \( \psi(x) \), one can derive the populations of the carriers within the junction. A typical example is shown in Figure 34, where populations for electrons and holes have been calculated for a typical 400nm i-layer a-Si:H, which is illuminated from the p-side under AM1.5G solar radiation. The carrier profiles are shown for two cases: short-circuit and open-circuit conditions. As shown the electron minority carrier concentration is significantly higher than the hole one, since the incoming light is directed from the p-side to the n-side. However, increasing bias gives rise to minority populations and the effect is gradually negated.

### 3.3.3. Poisson Equation

In addition to the continuity equation, Poisson’s equation must also be satisfied. This essentially is Maxwell’s first law. According to this equation the electric potentials is related to the charge density which gives rise to it. Its mathematical expression [78] is given below:

\[
\frac{d^2\psi}{dx^2} = -\frac{\rho_S}{\varepsilon_s} \quad \text{or} \quad \frac{dE}{dx} = \frac{\rho_S}{\varepsilon_s}
\]

(47)

It should be noted that \( \psi \) is the electrical potential across the junction, \( E \), the electric field and \( \rho_S \) is the local space charge density equal to:

\[
\rho_S(x) = -q \cdot [n(x) - p(x) - \rho \tau(x)]
\]

(48)

The charge, \( \rho_t \), represents the local trapped charge and equals to:

\[
\rho_t(x) = n_t(x) - p_t(x) + N_A^- (x) - N_D^+(x)
\]

(49)

The density of localized states and their distribution through the band gap are represented by two exponential distributions of tail states [63]. \( N_A^- \) and \( N_D^+ \) are the concentrations of the ionised donors. The concentrations of trapped carriers \( n_t \) and \( p_t \) are given by the expressions:

\[
n_t(x) = \int_{E_c^d}^{E_v} g_A (E) dE + \frac{n(x)}{n(x) + C \cdot p(x)} \int_{E_c^d}^{E_v} g_A (E) dE
\]

(50)

\[
p_t(x) = \int_{E_c^d}^{E_v} g_D (E) dE + \frac{p(x)}{n(x) \cdot C + p(x)} \int_{E_c^d}^{E_v} g_D (E) dE
\]

(51)
The energy, $E$, dependent densities of the acceptor-like and donor-like localised states are symbolised as $g_A$ and $g_D$ respectively. The ratio of the charged to neutral capture cross section $C = \sigma_C / \sigma_N$ is significantly higher than unity, since $\tau_n^+ \tau_p^- \ll \tau_{n,p}^0$ [93]. The ratio may vary in literature from 80 [66] to 500 [94]. Most scientists though estimate the ratio to 100 (e.g. [29], [63], [93], [95]). The electron and hole trap quasi-Fermi levels for acceptor-like states are given as [96]:

$$E_m^a = E_C + k \cdot T \cdot \ln \left( \frac{n + C_p}{N_C} \right)$$  \hspace{1cm} (52)

$$E_p^a = E_V - k \cdot T \cdot \ln \left( \frac{p + n / C}{N_V} \right)$$  \hspace{1cm} (53)

For donor-like states the expressions for electron and hole quasi-Fermi levels are:

$$E_m^d = E_C + k \cdot T \cdot \ln \left( \frac{n + p / C}{N_C} \right)$$  \hspace{1cm} (54)

$$E_p^d = E_V - k \cdot T \cdot \ln \left( \frac{p \cdot C + p}{N_V} \right)$$  \hspace{1cm} (55)

### Table IV: List of quantities used for electrical simulations

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C$</td>
<td>$100$ [29], [63], [93], [95]</td>
</tr>
<tr>
<td>$N_C$</td>
<td>$10^{18}$ cm$^{-3}$ [29], [79]</td>
</tr>
<tr>
<td>$N_V$</td>
<td>$10^{18}$ cm$^{-3}$ [29], [79]</td>
</tr>
<tr>
<td>$E_g$</td>
<td>$1.72$ eV [29], [63]</td>
</tr>
<tr>
<td>$E_A$, $E_D$</td>
<td>$50$ meV [29], [27]</td>
</tr>
<tr>
<td>$E_{mc}$</td>
<td>$65$ meV [27], [63]</td>
</tr>
<tr>
<td>$K$</td>
<td>$3 \cdot 10^{-16}$ cm$^3$ eV$^{-1.5}$ [63]</td>
</tr>
<tr>
<td>$g_{\min}(0)$</td>
<td>$10^{15}$-$10^{16}$ cm$^{-3}$ eV$^{-1}$ [27], [63]</td>
</tr>
</tbody>
</table>

$N_C$ and $N_V$ are the densities of states in the conduction and valence bands. $E_C$ and $E_V$ are the energies corresponding to the bottom of the conduction and top of the valance with the band-gap, $E_g = E_C - E_V$.

The acceptor-like and donor-like defect localised state densities $g_A$ and $g_D$ are given as:

$$g_D(E) = g_{D_{\min}} \exp\left[-\left(E - E_{m_D}\right)/E_D\right]$$  \hspace{1cm} (56)

$$g_A(E) = g_{A_{\min}} \exp\left[\left(E - E_{m_A}\right)/E_A\right]$$  \hspace{1cm} (57)

The quantities $E_A$ and $E_D$ are the so called characteristic energy slopes of the exponential distributions of acceptor-like and donor-like localised states. $E_{mc}$ is the energy difference between the minimum in the density of states and the conduction band. The quantities $g_{A_{\min}}$ and $g_{D_{\min}}$ are assumed to equal $g_{\min}/2$ [63]. According to Hack et al. [63] the defect density of states $g_{\min}$ equals:

$$g_{\min}(N) = g_{\min}(0) + K \sqrt{N / g_{\min}(0)}$$  \hspace{1cm} (58)
$N$ here is the dopant concentration and $K$ a material dependent constant. The numerical values, which are used in this thesis for the purpose of computation of the above mentioned formulas, are listed in Table IV.

\begin{figure}
\begin{subfigure}{0.45\textwidth}
\centering
\includegraphics[width=\textwidth]{fig36a}
\caption{Electrical potential assuming a constant and a varied electric field for short-circuit and open-circuit conditions.}
\end{subfigure}\hfil
\begin{subfigure}{0.45\textwidth}
\centering
\includegraphics[width=\textwidth]{fig36b}
\caption{J-V characteristics corresponding to constant electric field and varied electric field distributions under dark and light (AM1.5G) conditions.}
\end{subfigure}
\end{figure}

Solving the Poisson equation allows the calculation of the electrostatic potential across the junction. It should noted that assuming a constant electric field may be a fair approximation for low voltages, but as applied positive voltage increases the potential strongly deviates from the linearity occurring at short-circuit conditions exhibiting an s-like behaviour (Figure 36,a). The impact of these deviations is demonstrated in Figure 36, b with respect to J-V characteristics of a 400nm i-layer a-Si:H solar cell, whose behaviour under dark and light conditions is calculated for a constant and varied electric field profile. Therefore, a linear potential approximation may be sufficient to estimate the current flow of a-Si:H solar cells under short-circuit conditions, but it is not valid for evaluating its performance. As it is shown in Figure 36, b the current differences between the two modelling approaches may rise up to 10mA/cm$^2$ at open-circuit conditions. Thus, it is considered significant factor for evaluating the performance of the cells. For this is the reason, in this work, the potential is calculated using Poisson’s equation rather than using a linear approximation.
3.3.4. Recombination Statistics

Recombination of electrons and holes is a process by which both carriers vanish by means of electron-hole transitioning between the valance and the conduction band. An electron occupies - through one or multiple steps - the empty state associated with a hole. Both carriers eventually disappear in the process [97]. The energy difference between the initial and final state of the electron is released either as photon (radiative recombination) or a phonon (non-radiative recombination). Recombination processes can be classified in direct and indirect, with the first dominating in semiconductors with a direct band-gap [78]. Indirect recombination is expressing recombination via recombination centres, such as dangling bonds, and mainly occurs at indirect band-gap semiconductors. Amorphous silicon however does not have well defined band structure, and therefore both may occur. In practice the main recombination mechanism in a-Si:H solar cells is dangling bond recombination [98].

Figure 37: Schematic representation of different recombination mechanisms; Direct, trap-assisted SRH and dangling-bond Hubin-Shah recombination. The trap-assisted SRH recombination occurs on a recombination state via a capture of an electron from conduction and a hole from valence. The Hubin-Shah dangling-bond recombination process may be triggered either by a hole capture (lifetime, $\tau_p^0$) or an electron capture (lifetime, $\tau_n^0$) by a neutral dangling bond. It is followed by a consequent capture of an electron (lifetime, $\tau_n^+$) or a hole (lifetime, $\tau_p^-$) respectively by this newly created charged dangling bond respectively, that neutralises the bond again.

When an electron makes a transition from the conduction band to the valence, or a hole from the valence to the conduction band, an electron-hole pair is annihilated (Figure 37). The mechanism described is also known as band-to-band recombination and is a one-step process in the sense there is only one action intervening. Band-to-band
recombination mechanism depends on the availability of electron and hole densities. The process rate is proportional to the product of \( n \) and \( p \), as given by the following formula [97]:

\[
R_{B-B} = \beta \cdot (n \cdot p - n_i^2)
\]

The quantity \( \beta \) is a material dependent constant and the subscript \( i \) indicates here, the intrinsic concentration. In thermal equilibrium, the recombination is negated, as the electron and hole populations equal \( n_i \). For low injection conditions \((p_n0 \ll n_n0\) and \(n_p0 \ll p_p0\)), such as solar radiation, the above mentioned formula reduces for electrons and holes respectively to:

\[
R_{p\ B-B} = \frac{p_n - p_n0}{\tau_{p\ B-B}} \tag{60}
\]

\[
R_{n\ B-B} = \frac{n_p - n_p0}{\tau_{n\ B-B}} \tag{61}
\]

Here \( \tau_{n\ B-B} \) and \( \tau_{p\ B-B} \) represent the electron and hole band-to-band recombination lifetimes. The numerical values of the band-to-band recombination lifetimes used in this work are listed on Table V.

<table>
<thead>
<tr>
<th>Table V: List of quantities used for the recombination functions in the electrical simulations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity</td>
</tr>
<tr>
<td>( \tau_{n\ B-B} )</td>
</tr>
<tr>
<td>( \tau_{n\ B-B} )</td>
</tr>
<tr>
<td>( \tau_n )</td>
</tr>
<tr>
<td>( \tau_p )</td>
</tr>
<tr>
<td>( \nu_{th} )</td>
</tr>
<tr>
<td>( \sigma_n0 )</td>
</tr>
<tr>
<td>( \sigma_p0 )</td>
</tr>
<tr>
<td>( \sigma_n^* )</td>
</tr>
<tr>
<td>( \sigma_p^* )</td>
</tr>
<tr>
<td>( N_{DB} )</td>
</tr>
</tbody>
</table>

Trap-assisted recombination is a two-step process. It occurs when an electron falls into a trap, an energy level within the bandgap caused by the presence of a recombination centre, such as a dangling bond, or a lateral deficiency. Once the trap is filled, it cannot accept another electron. The electron occupying the trap, in a second step, falls into an empty valence band state, as shown in Figure 37. The statistics of this recombination process were introduced by Shockley, Read and Hall (SRH) [99] and thus is referred to as SRH recombination. The trap-assisted SRH recombination is limited by the minority carrier density [100] and is a parallel process, in the sense that two recombination paths occur simultaneously. Its mathematical expression is given by the following formula [94]:
The quantities \( \sigma_n \) and \( \sigma_p \) are the trap assisted capture cross sections for electrons and holes corresponding to the trap assisted carrier lifetimes \( \tau_n \) and \( \tau_p \) respectively. \( N_t \) is the density of the recombination centres and \( v_{th} \) is the thermal velocity\(^1\) of the material. The population densities \( n_f \) and \( p_f \) represent the free electrons and holes.

Hubin and Shah et al. [66], [93], [100] have suggested an alternative explanation for trap assisted recombination with particular focus to the role of dangling bonds in amorphous silicon. According to this theory, dangling bond recombination in a-Si:H is a three-step process, which occurs via two recombination paths, and each of them is the product of two successive capture events:

1. Hole, \( h \), capture from a neutral dangling bond, \( D^0 \), which changes the state of the bond to positively charged, \( D^+ \), as given by the transition: \( D^0 + h \rightarrow D^+ \) (lifetime \( \tau_p^0 \), as shown in Figure 37). Consequently, an electron, \( e \), may be captured by this newly created positively charged dangling bond, \( D^+ \), neutralising it again, as given by the transition: \( D^+ + e \rightarrow D^0 \) (lifetime \( \tau_n^+ \) in Figure 37).

2. Electron capture from a neutral dangling bond, \( D^0 \), which changes the charge state of the bond into \( D^- \) via the transition \( D^0 + e \rightarrow D^- \) (lifetime \( \tau_n^0 \), Figure 37). The event is followed by a hole capture on this newly created negatively charged dangling bond, turning it again into a \( D^0 \), as given by the transition \( D^- + h \rightarrow D^0 \) (capture \( \tau_p^- \))

As a consequence, along both recombination paths, the process is limited by the carrier with the higher concentration, which is the majority carrier density [94]. In this work this mechanism of recombination will be called dangling bond recombination, \( R_{DB} \). Its mathematical expression is given as:

\[
R_{DB} = \frac{n_f \cdot p_f \cdot \sigma_n}{n_f^2 + p_f^2} \cdot v_{th} \cdot N_{DB} \quad \text{or} \quad R_{SRH} = \frac{n_f \cdot p_f}{n_f \tau_p^0 + p_f \tau_n^0}
\]

\[(63)\]

\(^1\)Thermal velocity is the velocity or thermal motion of the particles of a substance. The thermal velocity of a substance is equal to the measure of temperature of the substance (solid, liquid, or gas).
$N_{DB}$ is the dangling bond density, $\sigma_n^0$ and $\sigma_p^0$ are the capture cross sections of neutral dangling bonds for electrons and holes respectively. The quantities $\sigma_n^+$ and $\sigma_p^-$ is the capture cross section of the positively and negatively charged dangling bonds. The numerical values used in this work are listed on Table V.

![Figure 38: Variation of recombination distributions for a typical 400nm i-layer a-Si:H solar cell under AM1.5G solar radiation. The notations RDB, RSRH and RB-B correspond to dangling bond recombination as proposed by Hubin et al. [66], trap assisted SRH recombination [94] and band-to-band recombination [63] with numerical values listed in Table V.](image)

A numerical comparison of the different recombination functions occurring in a-Si:H solar cell: band-to-band, trap-assisted SRH and dangling bond recombination, is shown in Figure 38. The numerical values of the properties used for the calculations are listed on Table III and Table V. In this investigation, a typical 400nm i-layer a-Si:H solar cell was considered, which was illuminated under standard AM1.5G solar radiation. As it is shown, band-to-band recombination is several orders of magnitude lower than trap assisted SRH and dangling bond recombination, as typical band-to-band recombination lifetimes for amorphous silicon are significantly lower that the corresponding lifetimes for SRH and dangling bond recombination. Therefore the latter two recombination mechanisms are identified as the major mechanisms of current loss. However, dangling-bond and SRH recombination also differ. While the first dominates under a low voltage applied bias, especially close to the i-n interface (right side), the second increases noticeably in forward bias conditions with a maximum in the middle of the i-layer. A numerical example of the current losses corresponding to each recombination mechanism as a function of voltage is given in
Figure 39 for a 400nm i-layer a-Si:H solar cell. Noticeably, the numerical values of dangling bond recombination maximise towards the i-n interface, as the capture cross section of neutral dangling bonds for holes is significantly higher than the capture cross section for electrons (Table V). In this work, best agreement with experimentally measured $J-V$ characteristics was established assuming that the mechanism with the higher recombination rate will dominate in respect to i-layer position. In addition SRH recombination was essential to fit solar cell characteristics under increased forward bias, while dangling-bond recombination played a more important role in the short-circuit region. Therefore the approach used in this work, is semi-empirical as it does not solely depend on one recombination function for the purpose of determining dangling-bond, or trap assisted recombination. A detailed comparison against experimental measurements will be the subject of discussion in section 3.5.

Figure 39: Variation of recombination distributions for a typical 400nm i-layer a-Si:H solar cell under AM1.5G solar radiation. The quantities $R_{SRH}$ and $R_{DB}$ correspond to trap assisted SRH recombination and dangling bond recombination as proposed by Hubin et al. [66].
3.4. Numerical Solution

To analyse accurately a semiconductor structure not only a mathematical model is required to describe the device, but also an underlying solution of it. However, the system of differential equations described in 3.3 cannot be solved analytically; therefore a solution is required by the means of numerical computation. In this section the numerical approach, which is necessary to solve the system of differential equations presented in section 3.3, is considered.

3.4.1. Boundary Conditions

In order to achieve a meaningful solution, appropriate boundary conditions must be chosen. In subsection 3.2.1 the main assumptions used to establish a solution for a solar cell’s equivalent circuit were elaborated. The first approximation implies that the electron and hole concentrations at the p-i and i-n interface equal the donor and acceptor densities. It was viewed that this assumption is true for a-Si:H solar cells, and therefore can be used again without altering significantly the generality of the solution.

The latter can be expressed mathematically as follows:

\[ p(0) = N_A \]  
\[ n(W) = N_D \]

(64)  
(65)

\( N_A \) and \( N_D \) are the acceptor and donor concentrations at the p-type and n-type layers respectively. \( W \) is the i-layer thickness.

By definition surface recombination will dominate at the interfaces, because of the abrupt discontinuity of the lattice structure at the interface, a large number of localised states are introduced. These states are called surface states and greatly enhance the recombination at the surface region. For a low injection condition, the total number of carriers recombining at the surface per unit area is proportional to the number of carriers [78]. Therefore, it can be assumed that the minority currents are proportional to the total number of minority carriers recombining at the surface (e.g. [28], [62]):

\[ J_n = S_n(n(0) - n_{p0}) \]  
\[ J_p = S_p(p(0) - p_{n0}) \]

(66)  
(67)
The quantities $S_n$ and $S_p$ represent the surface recombination velocities for electrons and holes respectively. The numerical values used for the purpose of numerical simulations are shown on Table VI. For $S \to 0$ the interface behaves as a perfectly passivated surface, while for $S \to \infty$ the interface behaves as an Ohmic contact. Generally, the surface recombination velocity for holes at the i-n interface is higher than that of electrons at p-i interface, and is partially responsible for the asymmetry shown by the voltage-dependent quantum efficiency of the cells, which will be examined in section 3.5.

The equilibrium concentrations $n_{p0}$ and $p_{n0}$, under zero bias and no illumination, can be approximated by the mass action law:

$$p_{p0} \cdot n_{p0} = n_i^2$$  \hspace{1cm} (68)  
$$p_{n0} \cdot n_{n0} = n_i^2$$  \hspace{1cm} (69)

The voltage across the junction is considered to be the difference between the built-in potential, $V_{bi}$, and the applied voltage, $V$. The voltage drops caused by parasitic series resistances, such as the TCO resistance, should be also considered. Therefore the boundary conditions for the potential, $\psi$, could be written as:

$$\psi(0) = 0$$  \hspace{1cm} (70)  
$$\psi(W) = V_{bi} - (V - J \cdot R_s)$$  \hspace{1cm} (71)

The boundary conditions (64)-(68) are sufficient to provide a unique solution ($\psi$, $n$, $p$) to the system of differential equations (40), (41), (45)-(47).
3.4.2. Numerical Solution

The system of differential equations (40), (41), (45)-(47) may define the carrier transport within a semiconductor mathematically. However it is not solvable from a computational point of view, as the dependent variables \((\psi, n, p)\) are of greatly differing orders of magnitude. A system of scaled equations which is more rigorous computationally was suggested by DeMari [87] and further evolved by Selberherr et al. [101]. The scaling factors are listed on Table VII. Using the scaling factors of Table VII and multiplying equations (40) and (41) with \(-x_0/(q\cdot C_0\cdot D_0)\), equations (45) and (46) with \(x_0^2/(C_0\cdot D_0)\) and Poisson’s equation (47) with \(\varepsilon/(q\cdot C_0)\), one arrives at a scaled version of the equations, which is more suitable for the numerical solution:

\[
J_n = \mu_n \cdot n \cdot \frac{d\psi}{dx} - D_n \cdot \frac{dn}{dx} \tag{72}
\]

\[
J_p = \mu_p \cdot p \cdot \frac{d\psi}{dx} + D_p \cdot \frac{dp}{dx} \tag{73}
\]

\[
\frac{d}{dx} \left( D_n \cdot \frac{dn}{dx} - \mu_n \cdot n \cdot \frac{d\psi}{dx} \right) - R(\psi, n, p) + G(x) = 0 \tag{74}
\]

\[
\frac{d}{dx} \left( D_p \cdot \frac{dp}{dx} + \mu_p \cdot p \cdot \frac{d\psi}{dx} \right) - R(\psi, n, p) + G(x) = 0 \tag{75}
\]

\[
\lambda^2 \cdot \left( \frac{d^2\psi}{dx^2} \right) + n - p - \rho_t = 0 \tag{76}
\]

where \(\lambda\) equals:

\[
\lambda = \sqrt{\frac{V_t \cdot \varepsilon}{x_0^2 \cdot q \cdot C_0}} \tag{77}
\]

The equations described above, are still non-linear and coupled. Therefore, one needs to define a domain, essentially the simulation geometry of the device, which has to be partitioned into a finite number of sub-domains. In each of the sub-domains the solution can be approximated. In addition the differential equations need to be decoupled and replaced by algebraically linear equations, which describe the dependant variables in each of the sub-domains in a continuous manner. In this way one can obtain a large number of linearised equations, as many as the number of sub-domains, which can describe the system non-linearly and holistically. The system can be solved using the
finite differences scheme with the first and the last domain defined by the boundary conditions described in 3.4.1.

Assuming electron and hole mobilities remain constant within the domain of simulation, but also that the carrier concentrations, \( n \) and \( p \), the net doping concentration, \( \rho \), as well as the recombination and generation functions in the locality of each sub-domain behave linearly, a linear decoupled system of equations can be derived. This system of equation would be equivalent to equations (72)-(76). The derivation of the equations is beyond the scope of this thesis and can be found in literature dedicated to simulation analysis of semiconductor devices (e.g. Selberherr [102]). Therefore, the set of equations, which are in correspondence to equations (74)-(76) are only presented here in their final form:
\[
D_n \frac{\psi_{i+1} - \psi_i}{V_i} \exp\left(\frac{\psi_{i+1} - \psi_i}{2V_i}\right) - \frac{\psi_{i-1} - \psi_i}{h_i} \frac{n_{i+1} - n_i}{h_i} + \\
+ D_n \frac{\psi_{i-1} - \psi_i}{V_i} \exp\left(\frac{\psi_{i-1} - \psi_i}{2V_i}\right) - \frac{\psi_{i-1} - \psi_i}{h_{i-1}} \frac{n_{i-1} - n_i}{h_{i-1}} - \\
- \mu_n \left\{ \frac{n_{i+1}}{1 + \exp\left(\frac{\psi_{i+1} - \psi_i}{2V_i}\right)} \right\} n_i \frac{\psi_{i+1} - \psi_i}{h_i} + \\
- \mu_n \left\{ \frac{n_{i-1}}{1 + \exp\left(\frac{\psi_{i-1} - \psi_i}{2V_i}\right)} \right\} n_i \frac{\psi_{i-1} - \psi_i}{h_{i-1}} + \\
+ (G_i - R_i^{m-1}) \frac{h_i + h_{i-1}}{2} = 0
\]

\[
D_p \frac{\psi_{i+1} - \psi_i}{V_i} \exp\left(\frac{\psi_{i+1} - \psi_i}{2V_i}\right) - \frac{\psi_{i-1} - \psi_i}{h_i} \frac{p_{i+1} - p_i}{h_i} + \\
+ D_p \frac{\psi_{i-1} - \psi_i}{V_i} \exp\left(\frac{\psi_{i-1} - \psi_i}{2V_i}\right) - \frac{\psi_{i-1} - \psi_i}{h_{i-1}} \frac{p_{i-1} - p_i}{h_{i-1}} + \\
+ \mu_p \left\{ \frac{p_{i+1}}{1 + \exp\left(\frac{\psi_{i+1} - \psi_i}{2V_i}\right)} \right\} p_i \frac{\psi_{i+1} - \psi_i}{h_i} + \\
+ \mu_p \left\{ \frac{p_{i-1}}{1 + \exp\left(\frac{\psi_{i-1} - \psi_i}{2V_i}\right)} \right\} p_i \frac{\psi_{i-1} - \psi_i}{h_{i-1}} + \\
+ (G_i - R_i^{m-1}) \frac{h_i + h_{i-1}}{2} = 0
\]

\[
\lambda^2 \left( \frac{\psi_{i+1} - \psi_i}{2h_i} + \frac{\psi_{i-1} - \psi_i}{2h_{i-1}} \right) - (n_i - p_i - \rho_i) \frac{h_{i-1} + h_i}{2} = 0
\]
The carrier concentration gradients are required to solve the current density equations (72) and (73) and define the boundary conditions. Both are approximated using the expressions:

\[
\frac{dn}{dx}_{i+1/2} = \frac{\psi_{i+1} - \psi_i}{V} \cdot \exp\left(\frac{\psi_{i+1} - \psi_i}{2V}\right) - \exp\left(\frac{\psi_i - \psi_{i+1}}{2V}\right) \cdot \frac{n_{i+1} - n_i}{h_i} \quad (81)
\]

\[
\frac{dp}{dx}_{i+1/2} = \frac{\psi_{i+1} - \psi_i}{V} \cdot \exp\left(\frac{\psi_{i+1} - \psi_i}{2V}\right) - \exp\left(\frac{\psi_i - \psi_{i+1}}{2V}\right) \cdot \frac{p_{i+1} - p_i}{h_i} \quad (82)
\]

The notation \( -i \) in the above mentioned formulas denotes the value of the quantity \( n, p, \) or \( \psi \) in the locality of \( x_i \). The superscript \( -m \) indicates the level of the iteration. Equations (78)-(80) are fully discretised and therefore each can be solved individually with a finite differences scheme. For the purposes of the numerical solution a Gummel-Schrafetter scheme can be adapted [86], [102]. Initially Poisson’s equation is solved, assuming fixed quasi-Fermi levels. The calculated potential is substituted to the continuity equations, calculating new electron-hole distribution. The electron-hole distributions are substituted back to Poisson’s equation, and a new iteration loop begins. A flow chart of this iterative process is shown in Figure 41. Even though the system has been significantly simplified, in practice convergence cannot be achieved unless the maximum perturbation of the electrostatic potential for each iteration step is controlled and kept smaller than a manually defined value, \( \omega \).

\[
\max\left(\left|\psi_i^m - \psi_i^{m-1}\right|\right) \leq \omega \quad (83)
\]

Therefore the potential \( \psi_i^m \), which can be used for the calculation of the electron and hole populations in iteration step \( m+1 \)th, can be evaluated as:

\[
\psi_i^m = \psi_i^{m-1} + \omega \cdot \frac{\psi_i^m - \psi_i^{m-1}}{\max\left(\left|\psi_i^m - \psi_i^{m-1}\right|\right)} \quad (84)
\]
where the potential $\psi_i^m$ represents the unscaled potential as calculated by formula (80) in the $m^{th}$ iteration step.

![Flow chart]

Figure 41: Flow chart describing the iterative process of the numerical solution.

3.4.3. Robustness of Solution

As previously discussed the simulation geometry of the device is partitioned into a finite number of sub-domains, in which each of the carrier concentrations is assumed to vary linearly. However, as shown in Figure 34, the gradients of the electron-hole populations strongly vary close to the interfaces and remain relatively constant within the middle of the i-layer. Thus, the sub-domain distribution should be carefully chosen to reflect the gradient changes in the mesh distribution, as accurately as possible. On the other hand,
computing the gradient changes and redesigning the mesh at each iteration step can prove computationally demanding. In this work, the Sigmoid-function, abbreviated as S-function, has been chosen for the purpose of defining the vicinity of each of the sub-domains compiling the simulation grid. The S-function imitates the growth of a population, which at initial stage is approximately exponentially; then, as saturation begins, the growth slows, and at maturity the growth stops [103]. Mathematically, the S-function is expressed by the formula:

\[ P(t) = \frac{1}{1 + e^{-t}} \]  

(85)

where the population, \( P \), is a dependent variable receiving values between 0 and 1, \( t \) is an arbitrary independent variable that ranges from \(-\infty\) to \(+\infty\).

This behaviour is similar to the diffusion of free carriers into i-layers and therefore it can provide a fair estimation of the scaled sub-domain boundaries on \( x \)-axis, which also vary between 0 and 1. A comparison between an equidistant and an S-like distributed mesh is shown in Figure 42, as an example for 200 points.

![Figure 42: Comparison between equidistant and s-like mesh distribution of points shown here as an example for 200 points.](image)

When the mesh is compiled by a sufficient number of points, the approximation of linearity of the \( n \) and \( p \) populations within the mesh sub-domains holds and convergence of the solution is established. As a result, the current density flowing within the device stabilises to the proximity of a value which should also be insensitive to any further increase of the number of points congregating the mesh. This is a means of proving the
integrity of the numerical solution and can be used to compare different mesh distributions compiled by a number of points, N, and draw conclusions for their adequacy. Figure 43 displays the modelled current density flowing through a 400nm i-layer thickness a-Si:H solar cell, which is illuminated under AM1.5G solar radiation under short circuit and open circuit conditions. For the purpose of the numerical simulations two different point distributions were assumed, equidistant and s-like, with varying number of points, N. For the reasons discussed in the previous paragraph, an equidistant mesh seems inadequate, as the system shows slow convergence for both bias conditions. Specifically, the modelled current density seems heavily dependent on the point density, even for increased point densities (N>300) and the result is greatly influenced by the number of points N. On the contrary an S-like mesh distribution is more robust, as convergence is established rapidly for N>200 for any range of voltages varying from short-circuit to open-circuit conditions. It should be noted that for short-circuit conditions an increase of the number of points N>500 for the equidistant mesh shown similar results with the S-like mesh with 200 points. In addition increasing the number of points to more than 500 for the s-like mesh may introduce problems. The points close to the vicinity of p-i and i-n interfaces will differ for less than 10^{-16} [a.u.], while estimating the derivative may introduce errors, as computing issues arise. In practice the simulation started to become unstable for more than 800 points for the s-like distribution. However, increasing the number of points may substantially increase the simulation time. For this reason, the number of points in the simulations is set to 200, in order to guarantee convergence and computationally effectible run-times for the simulation.

Figure 43: Dependence of convergence of the electrical model on the number of points and the mesh distribution for: (a) short-circuit, (b) open-circuit conditions, as shown here for a typical a-Si:H solar cell of 400nm i-layer illuminated under AM1.5G solar radiation.
3.5. Comparison of the opto-electrical model with experimental measurements

In this section the results of the optical model introduced in chapter 2 and the detailed semiconductor modelling presented in chapter 3 are compared with experimental measurements in terms of current density-voltage, $J-V$, and quantum efficiency, $QE$, characteristics. The comparison between the measured and the simulated $J-V$ and $QE$ characteristics is used to provide a validation basis for the model.

3.5.1. Case of Study

The $J-V$ characteristics of three cells of 250nm, 400nm and 600nm i-layer thickness were experimentally measured in the laboratory of IMT Neuchâtel. Varied i-layer thickness was chosen here, because it is known to have a strong influence on the optical absorption, the magnitude of the electric field and free carrier recombination. Hence, it has a very interesting influence on the performance characteristics of the cells.

The number of the independent parameters is significant, and therefore it is challenging to be accurately defined for every case individually. Thus, all the values for the parameters used in this work, are generic and can be commonly found in the literature. For this reason, it is unjustified claiming the chosen set of parameters is able to characterise uniquely each of the cells and to an extent present an accurate reproduction of its behaviour. As scientists have shown for similar models, e.g Krč et al. [26], Hack et al. [63] etc, modelling parameters can have a direct influence on a-Si:H solar cell behaviour. Hence, the accuracy of the model remains subjective to the accuracy of the input data, while, a thorough sensitivity analysis of all modelling parameters is required to claim a validation has been achieved. This examination though aims to study the performance of the cells under different spectral conditions and model their effects on performance, rather than holistically analyse every parameter of the a-Si:H solar cell modelling universe.

The exact structure of the cells is estimated to be of 1mm Glass / 500nm ZnO TCO layer / 10nm μc-Si p-layer / a-Si:H i-layer / 10nm μc-Si n-layer / 400nm: ZnO-Ag buffer layer-back reflector. The dopant concentration at the p$^+$-type and n$^+$-type degenerate
Seminiconductors is known to be at the order of $10^{18}$ cm$^{-3}$. The area of the samples is 1.2 cm$^2$ at all cases. The complex refractive index of the materials used in the simulations has been published by Springer et al. [31]. All the additional optical parameters for the purpose of the opto-electrical modelling are identical to the values, which were previously presented in chapters 2 and 3. In order to determine the values of parasitic resistances a method based on Merten’s model for the voltage-dependent photocurrent, was used as described in section 3.2.1. The experimental $J$-$V$ measurements together with their corresponding $J$-$V$ fittings are shown in Figure 44. The extracted values of the parasitic resistances are shown on Table VIII and will be used in the electrical simulations. It should be noted that all cells show excellent electrical behaviour, which is viewed by their low ohmic extracted series resistances and relatively high shunt resistance.

### Table VIII: Values of parasitic resistances extracted, and used in the electrical simulations

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Cell Thickness [nm]</th>
<th>Value [Ω/cm$^2$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_S$</td>
<td>250</td>
<td>1.729</td>
</tr>
<tr>
<td>$R_P$</td>
<td>250</td>
<td>455.49</td>
</tr>
<tr>
<td>$R_S$</td>
<td>400</td>
<td>1.579</td>
</tr>
<tr>
<td>$R_P$</td>
<td>400</td>
<td>568.63</td>
</tr>
<tr>
<td>$R_S$</td>
<td>600</td>
<td>1.685</td>
</tr>
<tr>
<td>$R_P$</td>
<td>600</td>
<td>718.81</td>
</tr>
</tbody>
</table>

Figure 44: Measured $J$-characteristics for three a-Si:H solar cells of i-layer thickness 250nm, 400nm and 600nm and their corresponding Merten’s equivalent circuit model fittings.
3.5.2. Comparison against \textit{EQE} and \textit{J-V} characteristics

In this section the modelled external quantum efficiencies (\textit{EQE}) of the three cells described above are compared with experimentally obtained \textit{EQEs}. To do so, firstly the devices were characterised optically and the generation profiles were computed under AM1.5G radiation. Secondly, the electrical behaviour of the cells was determined. This was done by calculating the collection rate of the photogenerated carriers at the device terminals, i.e. quantum efficiency and \textit{J-V} characteristics. No temperature variations were considered here as the focus is on laboratory measurements and temperatures are controllable within such an environment.

![Figure 45: Measured and modelled quantum efficiency curves for three a-Si:H solar cells of different i-layer thickness: 250nm, 400nm and 600nm.](image)

Best agreement in the front 380-450nm wavelength region was established by tailoring the p-layer to 9nm in the optical calculations. The estimated thickness is in the range of values, which have been typically used to simulate a-Si:H solar cells, e.g. Bruns et al. [29] have assumed a 10nm p-layer thickness and Zeman et al. [38] a 9nm one. Assuming high interfacial roughness at the back reflector was essential to successfully fit the characteristics at longer wavelengths, namely 560-800nm region ($\sigma_{rms}=50$nm). This value is also justified as it is similar with the value, which Springer et al. [31] and Krč et al. [26] have assumed in their calculations.
In Figure 45 the measured and modelled $EQE$s are being compared. It is shown that the model can realistically reproduce the measured $EQE$s assuming typical values for the properties characterising the a-Si:H solar cells, which are available in literature. At this point it should be emphasised that the presented $EQE$ modelled characteristics have not been produced by any kind of fitting procedure to match the measured data, since the original values of the assumed data have been used. Therefore, it cannot be claimed that the shown general agreement between the modelled and the measured behaviour validates the model, since most of the parameters used for the modelling have not been experimentally measured for the given set of solar cells. However, the computed characteristics show that the model can reproduce realistically the spectral response of a-Si:H assuming typical values for the opto-electrical properties of a-Si:H solar cells.

![Figure 46: Measured and modelled $J$-$V$ characteristics for three a-Si:H solar cells of different i-layer thickness: 250nm, 400nm and 600nm. The excitation spectrum in this case is the standard terrestrial AM1.5G radiation.](image)

The measured and modelled $J$-$V$ characteristics are shown in Figure 46. The inclusion of parasitic resistances shown on Table VIII was essential to show an agreement with the experimentally measured characteristics. Best agreement at open circuit voltage $V_{oc}$ conditions was achieved by calibrating the built-in potential. The variations of the built-in potential $V_{bi}$ were small, 1.205V for the 250nm cell, 1.198V for the 400nm cell and 1.177V for the 600nm cell. It should be noted that these results are based on the same set of input used for modelling the $EQE$ of the device. The model shows a good agreement with the experimental measurements for all three cells. However, the performance of the 600nm i-
layer cell seems to be underestimated in the region of 0.4-0.7V. This can possibly be attributed to a number of reasons such as a non-ideal estimation of the electrostatic potential distribution, or an overestimation of the recombination. Therefore, it is understandable why such deviations may occur.

3.6. Conclusions

In this chapter different methods were used to model the electrical collection of a-Si:H solar cells. Equivalent circuit modelling is the simplest and easiest to compute method, but it is not appropriate for modelling the behaviour of a-Si:H solar cells. Specifically, the distribution of the potential within the device is not linear, as at best such models assume. In addition the estimation of photogenerated carriers cannot be quantified by a bulk term, but it is a complex function, which needs to be characterised by the means of optical modelling, as explained in chapter 2. Furthermore, as the aims of this work is to examine the behaviour of the device under varied spectral conditions, it is unfeasible to do so based on equivalent circuit modelling.

On the other side a detailed semiconductor modelling may be suitable for describing the effects of spectral changes on a-Si:H solar cell performance, but in the majority of cases it is impractical, as it requires a significant amount of computation and is dependent on large number of input parameters. In this work a comprehensive electrical model has been developed, which is able to model the specifics of a-Si:H solar cells such as the dangling bond recombination and the variation of the electrostatic potential distribution within the i-layer. Crucially, photogenetation here is defined by a thorough optical model that takes into account the device structure details and its variation of optical absorption within a wavelength band. The latter is of vital importance, as the conjunction of the two models essentially enables the characterisation of the behaviour of the device under different optical excitation conditions. The latter is a tool to examine the performance of optical a-Si:H solar cells under varied indoor and outdoor conditions, which will be examined in the next following chapters.
Chapter 4 – Effects of Spectral Variation on Indoor Measurements

4.1. Introduction

In the previous chapters an opto-electrical model was designed, which is able to simulate the behaviour of a-Si:H solar cells under different illumination conditions. In this chapter the model will be employed to study the effects of different illumination spectra on the indoor performance evaluation of a-Si:H solar cells. The performance evaluation is carried out by assessing the power rating of the devices, which is given by the efficiency of the PV modules and the total area of these used in the system.

The power rating of photovoltaic devices decides the value of the product and thus is of utmost importance in the value chain. It is typically determined by a solar simulator measurement. The spectrum of these solar simulators should resemble the standard terrestrial AM1.5G radiation [56], [104]. In reality, though, their spectrum deviates significantly from this ideal spectrum. The deviations can be in the range of ±25% in a given spectral band and still meet the highest classification of solar simulators [22, 23]. The difference for solar spectrum is normally accounted for by carrying out a spectral mismatch correction [105], which works well for correcting current differences. In production, this is normally accounted for by calibrating the solar simulator, which is satisfactory as long as the assumption holds that all devices are identical.

The irradiance level in a simulator is mostly measured with reference cells. These are calibrated devices, mostly based on c-Si technologies (e.g [106, 107]). The calibration of the test device based on the responsivity of the reference cell at short-circuit conditions is generally accurate, since the band-gap of c-Si is smaller ($E_{g,c-Si}=1.12eV$) to a-Si ($E_{g,a-Si}=1.72eV$). Therefore, a current agreement may be established for short-circuit conditions, providing the spectral response of the measured and test device are known. Even so, c-Si reference cells are based on p-n junctions, whose electrical behaviour, as discussed in chapter 3, differs from p-i-n a-Si:H solar cells. It has been shown ([29, 108]) that there is a secondary effect on the fill factor for amorphous silicon...
devices. This generally is not considered and introduces an uncertainty into the measurement process. This effect has been attributed to the voltage dependence of the quantum efficiency of amorphous silicon photovoltaic devices [29]. As a result, a device may be calibrated correctly under short-circuit conditions, but this calibration does not hold for other bias conditions. Therefore, a measurement of the $J-V$ characteristics of a device will inherit a bias dependent deviation.

As briefly discussed in chapter 1, different solar simulators may have significantly different illumination spectra. The effects are further augmented with the use of LED solar testers\(^1\), which have been introduced recently [19-21], some of which are based on a single colour LEDs only. It is shown in this work that this may increase the uncertainties further, if not implemented carefully. An additional difficulty in calibrating a-Si:H technologies is their metastable material properties. Amorphous silicon is known to exhibit degradation after prolonged light soaking [24] or annealing due to high operating temperatures [67]. Both effects will have an effect on the voltage dependent quantum efficiency of the device. Therefore the device state should not been neglected.

In this chapter the performance of a-Si:H cells of varying i-layer thickness and level of degradation under different excitation spectra is probed. The investigation is achieved using the models, which were elaborated in chapters 2 and 3. The selected spectra include those of class A, B and C solar simulators, light-emitting diodes (LEDs), Tungsten and the standard terrestrial AM1.5G radiation spectrum [56]. Cell performance is examined here in combination with different levels of degradation and i-layer thickness because both are expected to have a strong influence on the magnitude of the electric field, free carrier recombination and hence the voltage dependence of the photocurrent. The investigation shows that the performance of the cells depends on the light source, but also the device state.

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\(^1\) Most devices do not meet the criteria set out in international standards [IEC60904-9] for solar simulators, hence the use of the term solar tester.
4.2. Parameterisation of the studied cells

In chapter 3 the modelled behaviour of three cells of i-layer thickness 250nm, 400nm and 600nm has been compared against experimental measurements. It was shown that the model can describe the behaviour of a-Si:H solar cells. A general set of parameters will be applied for all studied cases, in combination with different i-layer thicknesses and two degradation conditions; as prepared and degraded.

It was shown in chapter 2 that dangling bond density is important for recombination occurring within a-Si:H solar cells, and will influence the degradational state of the device. The mechanisms of this process have been attributed to increasing dangling bond density (e.g. [24], [67]). Scientists suggest ([30], [94]) that dangling bond density in a-Si:H usually varies between $10^{15}$-$10^{16}$ cm$^{-3}$ in hydrogenated amorphous silicon. In this work, the ageing was simulated by increasing the dangling bond density of bulk a-Si. The numerical values used in the frame of this work are shown in Table IX.

The simulated cells have a structure of 1mm Glass / 500nm ZnO TCO layer / 10nm µc-Si p-layer / a-Si:H i-layer / 10nm µc-Si n-layer / 400nm: ZnO-Ag buffer layer - back reflector. The dopant concentration at the p$^+$-type and n$^+$-type degenerate semiconductors is assumed to be $10^{18}$ cm$^{-3}$. The selected i-layer thicknesses have been 250nm, 400nm and 600nm, which are in the range of most commercial a-Si:H solar devices [27], but also in a range where device efficiency is significantly affected by degradation. Specifically, Yang et al. [110] have shown that degradation rate in a-Si:H cells increases monotonically with increasing i-layer thickness for devices with i-layer 200-800nm. Similar effects have been shown by Fantoni et al. [111], who has modelled the electrical behaviour of a-Si:H solar cells under degradation. In this work a direct correlation between i-layer thickness and degradation is established. Devices whose i-layer exceeded 400nm and have suffered degradation show their performance parameters significantly affected comparing to their as-prepared initial state. On the contrary devices that have also suffered degradation, but have an i-layer thickness close to 200nm show smaller deviations to their performance.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu_n/\mu_p$</td>
<td>$10^{29}$, [63]</td>
</tr>
<tr>
<td>$N_{DB, as, prepared}$</td>
<td>$10^{15}$ cm$^{-3}$ [30], [94]</td>
</tr>
<tr>
<td>$N_{DB, degraded}$</td>
<td>$7 \cdot 10^{15}$ cm$^{-3}$ [30], [94]</td>
</tr>
<tr>
<td>$R_S$</td>
<td>$2 \Omega$ cm$^2$ [109]</td>
</tr>
<tr>
<td>$R_P$</td>
<td>$1000 \Omega$ cm$^2$</td>
</tr>
</tbody>
</table>
parameters. This degradation mechanism is associated with bulk a-Si:H degradation and i-layer thickness, which is exactly the focus of this work.
Figure 47: Simulated distribution of light absorption in different layers of a-Si:H p-i-n solar cells for three different cells of i-layer thickness 250nm (a), 400nm (b) and 600nm (c). The specifics of the cells are detailed and labelled for each case.
The optical analysis of the studied cells was carried out based on the model described in chapter 2 and shown in Figure 47. In a manner similar to the results shown in chapter 3, thicker i-layer cells absorb more light, which becomes noticeable in the area of poorer absorption at wavelengths greater than 650nm. The same optical analysis is followed for both degraded and non-degraded devices. Strictly speaking dangling bond density will have an effect on absorption extending to wavelengths beyond amorphous silicon bandgap 1.72ev ($\approx 721$nm), as it was already mentioned in chapter 2. However the device quantum efficiency is relative poor in this region, therefore this does not significantly change the analysis laboured in this examination.

Figure 48: Modelled $EQE$ of the studied cells at 0V in as prepared and degraded state (a) and their corresponding simulated $J-V$ characteristics (b). The excitation spectrum used for the purpose of $J-V$ characteristics is the standard terrestrial AM1.5G radiation.
The contribution of the generation profile is analysed and converted into collected charge carriers, i.e. quantum efficiency and $J-V$ characteristics. The temperature has been set equal to standard test conditions (STCs) temperature (25ºC) [56]. Temperature variations are not considered here, since the examination focus is measurements obtained in the laboratory and temperatures are controllable within such an environment. The external quantum efficiency ($EQE$) in this examination corresponds to the response of the device at short circuit conditions (0V). For the simulations the STC AM1.5G light source was used as bias light. The modelled $EQE$ and $J-V$ characteristics are displayed in Figure 48. In the simulations the thicker i-layer a-Si:H cells show increased susceptibility to degradation rate, as caused by increased bulk dangling bond density. In agreement with the results illustrated in Figure 47, where the thickest i-layer cells showed higher light absorption, the 600nm i-layer cell exhibited the highest $J_{SC}$, followed by the 400nm i-layer cell. Interestingly, the situation has not been the same for the degraded state, where the thickest i-layer cell marginally exceeded the $J_{SC}$ of the thinnest i-layer cell (250nm). These results are in agreement with the experimental observations of Yang et al. [110] and Vorasayan et al. [69], who reported increased degradation for increased i-layer thickness of a-Si:H solar cells. In addition, as also shown in chapter 3, increased i-layer thickness is not beneficial for the fill factor\(^1\). Increased i-layer thickness results in a decreased $V_{OC}$. The later becomes even more noticeable in the degraded state, where the thinnest cell shows clearly the highest $FF$ as well as $V_{OC}$. The above mentioned effects, which are caused by either degradation and i-layer thickness, have been observed by other scientists (e.g. [110],[63]) and have been attributed to the following factors:

i) Increased collection lengths of thinner i-layer cells due to increased built-in electric field.
ii) The mean required photocarrier path, which is required for successful collection, is shorter in thinner cells because of the thinner i-layer thickness.
iii) Increased dangling bond density, which is observed in degraded cells, increases recombination and limits collection at the terminals of the device.

---

\(^1\)The fill factor ($FF$) is defined as the ratio of the actual maximum obtainable power, ($J_{MP} \times V_{MP}$) to the maximum theoretical power, ($J_{SC} \times V_{OC}$). The fill factor is commonly used as key parameter in evaluating the performance of solar cells.
All of these factors are augmented by increasing voltage as the electrostatic potential, \( \psi \), across the junction collapses, further decreasing successful collection, as shown in Chapter 3, Figure 36, (a).

### 4.3. Different light sources

The steady-state and flash solar simulators are widely used today in laboratories to characterise a-Si:H solar cells. The light source of both types is generally based on single lamp, whose spectrum is suitably tailored by the use of selective bandpass filters (e.g. UV [115], or IR [116] filters). Therefore, these light sources maintain a spectral distortion of the spectrum arising from their illumination source.

New technologies [19-21] based on LED sources have been introduced. The main advantage of these light sources is their longer lifetime than conventional high-intensity simulator bulbs, which reduces maintenance costs to a minimum. In addition LEDs can be controlled very accurately with a stable power output can be achieved within microseconds. However, as attractive LED solar simulators may be, their illumination spectrum consists of a narrow band of wavelengths, and therefore deviates strongly from the standard terrestrial AM1.5G radiation.

<table>
<thead>
<tr>
<th>Solar Simulator Spectrum</th>
<th>Class</th>
<th>APE [eV]</th>
<th>Standard Deviation [eV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>AM1.5G [56]</td>
<td>-</td>
<td>2.1389</td>
<td>0.356</td>
</tr>
<tr>
<td>Solar Simulator 1</td>
<td>A</td>
<td>2.1650</td>
<td>0.365</td>
</tr>
<tr>
<td>Solar Simulator 2</td>
<td>A</td>
<td>2.1487</td>
<td>0.359</td>
</tr>
<tr>
<td>Solar Simulator 3</td>
<td>A</td>
<td>2.1533</td>
<td>0.381</td>
</tr>
<tr>
<td>Solar Simulator 4</td>
<td>B</td>
<td>2.1279</td>
<td>0.363</td>
</tr>
<tr>
<td>Solar Simulator 5</td>
<td>C</td>
<td>2.2182</td>
<td>0.364</td>
</tr>
<tr>
<td>Blue LED, ( \lambda = 445\text{nm} )</td>
<td>-</td>
<td>2.7784</td>
<td>0.061</td>
</tr>
<tr>
<td>Red LED, ( \lambda = 640\text{nm} )</td>
<td>-</td>
<td>1.9267</td>
<td>0.054</td>
</tr>
</tbody>
</table>
As outlined above, there are indications that different spectra have different effects on the performance of a-Si devices which goes beyond that of a simple mismatch correction [105], [112]. This is investigated here using two very extreme spectra, two different LEDs, a blue ($\lambda = 445$nm) and a red ($\lambda = 640$nm) and also a number of illumination spectra typically used for measuring a-Si devices in the different laboratories. The selected spectra are of commercially available solar simulators of spectral class A, B and C [22]. The standard reference spectrum AM1.5G is taken as defined in [56]. Also included is the spectrum of a tungsten halogen light, as these are also used in some laboratories to characterise a-Si:H based devices. Both Tungsten and LEDs spectra may be inappropriate for the purpose of simulating the standard terrestrial spectrum, but they are used in some instances nevertheless. The comparison of the
above mentioned light sources normalized to spectral irradiance spectra in 380-800nm region is given in Figure 49.

The average photon energy (APE) number, as defined by Betts et al. [113], is used to compare different spectra. Characterising spectra with their APE may simplify spectral differences and may not reflect all features seen in indoor calibrations, but allows a characterisation of the incident spectrum with a single number. A comparison of the used spectra in terms of APE and its standard deviation is given in Table X. Together with APE, the underlying generation profiles of each light source are used to compare sources for the case of 600nm i-layer cell (Figure 50). The cell with the thickest i-layer was selected here for instructive reasons, since it can illustrate the differences of the illumination sources more profoundly. In contrast with APE the generation profile may offer more information on the light source, but its evaluation has inevitably higher complexity, as it is sensitive to the device structure. In addition, its calculation involves optical modelling, which in turn requires the knowledge of a significant number of input parameters as discussed in chapter 2.

Figure 50: Illustration of the underlying generation profiles used in the simulations for the case of the 600nm i-layer cell. The profiles shown here correspond to the illumination spectra of class A solar simulators (a) to class B, C, Tungsten and two LED spectra (b).
The generation rates illustrated in Figure 50, can be better understood in combination with the $APE$ of the sources shown on Table X. Generally, lower $APE$ spectra cause a higher photogeneration of carriers at the rear region of the i-layer ($i$-$n$ interface), while higher $APE$ spectra show higher excitation at the front region ($p$-$i$ interface). The effect can be attributed to high energy radiation being absorbed more strongly in the bulk layer. The opposite holds for spectra with lower energy. This can be seen comparing the class A solar simulator 1, 2 and 3 and class C solar simulator 4 excitation profiles with the one of standard terrestrial AM1.5G radiation. As these solar simulators have higher $APE$ than the AM1.5G (Table X), it is understandable why their generation profiles are significantly lower at the back of the device. The same is apparent in the profiles of the blue and red LED (Figure 50), as well as the Tungsten light sources. Solar simulator 5 has a higher $APE$ than the other simulators but also has a high red contribution, as seen by its increased absorption at the rear side of the device. In addition focusing at the first 10nm of the i-layer and comparing its behaviour with the class A solar, one can observe that indeed this solar simulator has higher $APE$ since its generation rate decays faster (Figure 51). This rather peculiar behaviour can be explained with the spectrum of solar simulator 5 shown in Figure 49. This simulator contains two non-negligible peaks, which are rich in blue and red energy. Therefore its overall generation profile may resemble characteristics observed in both “blue-rich” and “red-rich” spectra, despite its overall high $APE$. 

![Figure 51: Comparison of normalized spectra used in the simulations. It is shown that the class C solar simulator causes a poorer generation at the first 10nm of the i-layer depth profile comparing the class A solar simulators.](image)
4.4. Effects of solar simulator spectra on the performance evaluation

In this section a performance comparison of the a-Si:H solar cells, which were presented in 4.2, under the illumination of the light sources examined in 4.3, is carried out. In most laboratories, the solar simulator intensity level is calibrated based on the performance of a reference cell under short-circuit conditions, effectively correcting most errors which arise at 0V. For this reason, the intensity level of all light sources in the simulations is calibrated to produce the same short-circuit current density as the standard terrestrial AM1.5G radiation for every cell and degradation state. Strictly speaking, this is equivalent with calibrating the spectral irradiance of each spectrum, so the number of collected photo-carriers under short-circuit conditions matches the collected photo-carriers under standard terrestrial AM1.5G excitation. Since the input photon flux and consequently the intensity of the light source do not matter in the calibration, it would be inappropriate to compare the efficiency of each device under different excitation sources. Hence, the performance comparison of the a-Si:H solar cells under different light sources, which is held here, is done in terms of the open-circuit voltage, $V_{OC}$, the maximum power output and the fill factor, $FF$. The short-circuit current density, $J_{SC}$, is always the same and corresponds to $J_{SC}$ of the AM1.5G radiation.

Figure 52 shows small, but noticeable changes in the performance parameters of the same devices under different excitation spectra. It is shown that high class solar simulators realistically do not suffer from significant secondary effects and effects in the measurement calibration will dominate. The introduced deviations in most cases do not exceed 0.3% for the power output and fill factor ($FF$). It is shown that red shifted spectra, e.g. the Tungsten-Halogen or the red LEDs show lower performance characteristics much more significantly with deviations exceeding 1.5%. Spectra which have a blue-shift on the other side, like the blue LED or in a lesser degree solar simulator 5, tend to show higher device performance. Such behaviour can also be observed for the solar simulator 1, which is relatively “blue shifted” (Table X ).
comparing to the other class A solar simulators. Degradation, expressed here as a fixed higher density of dangling-bonds, has a considerable effect on measurement uncertainty, as the deviations were doubled in most cases. The only deviation from this observation has been the 600nm i-layer cell, which showed a decrease in the deviation evaluation for the case of the blue and the red LED.

Figure 52: Difference of the simulated performance parameters under different excitation spectra to STC performance for cells of 250nm, 400nm, 600nm i-layer thickness in as prepared and degraded state. In all cases the J-V curves were calibrated to match $J_{SC}$ of standard test conditions.

The results presented in Figure 52 show that the i-layer thickness did not affect the measurement uncertainty significantly under the examined solar simulator spectra. However, the results shown here do not suffice to draw a conclusion about the impact of
i-layer thickness and varied illumination spectra on a-Si:H performance evaluation. As previously stated the investigation was carried out assuming a calibrated $J_{SC}$ condition based on STC $J_{SC}$ flow. This assumption may screen several effects, as the input photon flux is not the same for all cases.

For this reason the solar simulator spectra were also calibrated to match the input intensity of standard terrestrial AM1.5G radiation in the 380-800nm spectral region. The latter may not have a practical importance, as it is not used as standard in laboratories, but has a particular importance, as it can escalate the magnitude of the effects and provide a better understanding of the impact of spectral effects on
performance. Additionally, it is used here as an example to indicate the sensitivity of the performance evaluation on the selected conditions, because choosing a different spectrum as a basis for comparison will result in different performance evaluations even under the same light intensity. The practical difficulty in this case, is while the AM1.5 spectrum extends from 0nm to 4000nm, most solar simulators have much narrower profiles. Therefore, it was decided to take into account in the calibration only the wavelengths, which contribute to current generation for the a-Si:H solar cells. Specifically, in the 380-800nm wavelength window the AM1.5G radiation has an intensity of 555.38W/m², which all spectra were calibrated to match. Then the performance of each cell under STCs, both in the as-prepared as well as the degraded conditions, was compared with the performance under the examined solar simulator spectra. The results of the simulations are shown in Figure 53.

The results shown in Figure 53 show a direct correlation between the $FF$ and the excitation spectrum. In particular, bluer spectra show a beneficial influence on the $FF$, while redder spectra weaken it. Interestingly, the dominant effect for determining the $J_{SC}$ seems to be the highest photon flux and not the energy of the photons, as the highest $J_{SC}$ was recorded for red LED excitation and the lowest for the blue LED light source. Since all spectra here were calibrated by their total light intensity, high energy spectra will contain lesser photons, and therefore cause a lower current. Nevertheless, the presented results are a strong indication that the effects cannot be fully understood only from their spectrum inclination towards blue, or red. Interestingly, spectra which have a “redder” APE, such as the red LED and the tungsten light sources, show an opposing influence on $J_{SC}$, maximum power output and $V_{OC}$. A similar inconsistency was simulated for solar simulators 3 and 5, which both appear to be “blue-shifted” (Table X), but show an opposing influence on the performance parameters, but the FF. Regarding the i-layer thickness the results again do not show a significant influence on the magnitude of the deviation for most light sources.

All the examined spectra are continuous and contain wavelength narrow bands of unequal intensities. Therefore, although they can provide a general understanding of the effects, they are not suitable for providing a separation of the wavelength dependency of the performance assessment in a-Si:H solar cells. In order to separate spectral effects
and understand their impact quantitatively, an examination of monochromatic excitation sources is required.

4.5. Effects of monochromatic spectra on the performance evaluation

In order to separate the wavelength dependency of the effects examination of monochromatic excitation spectra is required. The calibration criteria selected are the matching current density under short-circuit conditions and the matching light intensity under STCs. The first because it is the standard calibration procedure used in the laboratories and hence, it can identify possible deviations arising in the performance evaluation. The second is selected because it can investigate the effect of spectral variation under a different point of view, and also show the relevance of the selected conditions on the performance assessment of the device.

40 monochromatic illumination spectra were chosen to generate an understanding of the effect of wavelength on performance parameters. The wavelengths range from 390nm to 780nm. The sources were simulated by a Gaussian function with a full width at half maximum equalling to 1nm. The centre of the Gaussian peak, which is essentially the light source peak, varied from 390nm to 780nm with a fixed interval of 10nm.

In Figure 54 it is shown that there exists a correlation among the magnitude of the deviations with i-layer thickness, degradation and photon energy. The performance of a-Si:H cells show higher values for blue light sources (400-500nm). The vales of the performance parameters are increasing and reaching its peak in the yellow-green region (500-590nm). The deviation decreases progressively in the yellow-orange region (570-660nm) until it becomes negligible. Performance is progressively decreasing in the orange (590-640nm), red (640-700nm) and infra-red regions (700-750nm). Furthermore, thicker i-layer devices are prone to higher deviations. This does not necessarily mean that devices with thicker i-layer thickness will consistently exhibit higher deviations, but that the maximum possible performance deviations have been simulated for the thickest cell (Figure 54, e and f). This is also in agreement with the
results presented in section 4.4, where not necessarily the thickest cell exhibited the highest deviations.

Figure 54: Difference of the simulated performance parameters under different monochromatic excitation spectra to STC performance parameters for cells of 250nm, 400nm, 600nm i-layer thickness in as prepared and degraded state. In all cases the J-V curves were calibrated to match $J_{SC}$ of standard test conditions.

The level of degradation has also a strong effect on the observed deviations. Increased degradation resulted in higher maximum deviations, as shown here for the 600nm cell (Figure 54, e and f). The wavelength of the maximum possible deviation is consistently increasing with increasing i-layer thickness, but also with the level of degradation. It is now also understood that degradation will have an impact on the maximum possible deviations. However, it is possible for a device to exhibit lesser deviations in the degraded state, such as the 600nm i-layer cell for the red LED light source (as shown in
Figure 52, e and f), because the performance evaluation of a device remains relative to the light source. This is the reason the 600nm i-layer cell exhibited smaller performance deviations than the other cells. In this case, the red LED examined in the previous section had its illumination peak situated at 640nm (Figure 54, f), which is very close to the wavelength area, where the degraded 600nm i-layer device shows its minimum performance deviation.

Figure 55: Difference of the simulated performance parameters under different monochromatic excitation spectra to STC performance parameters for cells of 250nm, 400nm, 600nm i-layer thickness in as prepared and degraded state. In all cases the J-V curves were calibrated to match intensity of standard test conditions (555.38W/m²).

The effects of spectral variation of monochromatic light sources on performance assessment were also examined under the point of view of calibrated flux light intensity. The results of the simulations are shown in Figure 55. It is shown that indeed in terms of $J_{SC}$, maximum power output and $V_{OC}$ the best performance yield comes from photons
located in the orange spectra region (~600nm). Specifically there are two effects occurring, the first is that bluer spectra are beneficial for the $FF$; the second, redder spectra contain significantly more photons per unit energy. Therefore, since in this examination the excitation spectrum is weighted to match the intensity of the STC (555.38W/m$^2$) in the spectral region of 380-800nm, it is understandable why neither extreme blue, or red spectra show the highest performance evaluation. The main reasons behind this behaviour are:

(i) Short wavelengths ($\lambda<500$nm) may enjoy higher collection rates, but contain far less photons per Watt. In addition a considerable amount of them is absorbed by the TCO and the front inactive layers. Consequently the generated far electron-hole pairs are greatly reduced. Therefore the total generated current is reduced.

(ii) Long wavelengths ($\lambda>650$nm) may contain significantly more photons per Watt, but suffer from incomplete absorption and poor collection rates.

In view of the results shown in Figure 55, it is understandable why the red LED produces higher $J_{SC}$ and maximum power output, while the blue LED lower (Figure 53, e and f). The red LED ($\lambda=640$nm) is situated exactly at peak of $J_{SC}$, maximum power output curve, while the blue LED ($\lambda=445$nm) has its centre of excitation in a region where both these parameters show minimum values.

Nevertheless, the above mentioned behaviour of the performance parameters cannot be attributed to the spectral variations and the response of the device alone. Changes in sheer light intensity can also cause a similar behaviour due to the nature of the diode and its parasitic resistances. It is generally known for solar cells, that moderately low intensities are beneficial for the $FF$, as in conditions of moderate low excitation the ratio of the rectangles of maximum power output and theoretical power output reaches its maximum. This is shown below (Figure 56) in a simplified single diode model simulation of the $I-V$ characteristics a a-Si:H solar cell under varying light intensity. It is shown that decreasing short circuit currents, as caused by reduced light intensities correspond to progressively higher $FF$ values. At very low irradiances (<100W/m$^2$) though, the $FF$ is heavily affected by the shunt resistance, which is causing the $FF$ to
reduce steeply. In a similar manner high intensities also show progressively reduced FF, due to the role of the voltage-dependent photocurrent and the series resistance. Therefore, it cannot be neglected that both blue and red monochromatic light sources will produce lower $J_{SC}$ corresponding to spectral regions of low responsivity of the a-Si:H device (Figure 48). Consequently, lower $J_{SC}$ will also correspond to higher $FF$ values as shown in Figure 55.

![Figure 56: I-V characteristics (a) of an a-Si:H solar cell simulated with the single diode model for increasing light intensity (0-1200W/m$^2$). Variation of the $FF$ (b) for the same under the same variation of light intensity. It is shown that light intensities and the parasitic resistances have an effect on the $FF$; assuming no other secondary effects such as temperature, spectral variations, or voltage-dependent photocurrent. At low intensities the $FF$ is dominated by shunt effects, while the $R_s$ and the voltage dependent photocurrent plays a much more important role at higher intensities.](image)

4.6. Voltage dependent quantum efficiency and partial collection efficiency

In sections 4.4 and 4.5 it was shown that indeed a spectral variation will cause a non-negligible effect on the evaluation of photovoltaic performance of a-Si:H solar cells. What has not been made clear, however, are the reasons which are responsible for the deviation of performance. In this section it will be shown that the above mentioned effects are occurring because there is a change in the spectral response of the device with increasing voltage. The primary quantity, which reflects the electrical response of a device for different photon energies and voltages, is the voltage-dependent external quantum efficiency ($EQE-V$) of a device. Therefore, it is used in this section to analyse
the spectral behaviour of the device under different applied voltages ranging from short-circuit to open-circuit conditions.

The voltage dependent external quantum efficiency, \( EQE \), of a device illuminated by a monochromatic light source of wavelength \( \lambda \) and spectral irradiance, \( E_i \), under a light bias source and a voltage bias, \( V \), is given by the following formula:

\[
EQE(V, \lambda) = -\frac{J_{\text{bias},\lambda}(V) - J_{\text{bias}}(V)}{E_i} \frac{h \cdot c}{q \cdot \lambda} \quad (86)
\]

\( J_{\text{bias},\lambda} \), is the current density flowing the device under the combined illumination of the monochromatic excitation source and the bias light. \( J_{\text{bias}} \), is the current density flowing the device under the illumination of the bias light.

In Figure 57 the simulated \( EQE-V \) curves for the examined cells of 250nm, 400nm and 600nm i-layer thickness are shown in as-prepared and degraded state. The voltages here vary from short-circuit to the \( V_{OC} \), which corresponds to each device as shown in Figure 48, b. The selected bias light, which has been chosen, is the AM1.5G STC illumination. There is a systematic decrease of \( EQE \) with increasing voltage. Increasing bias will cause a progressive collapse of the internal electric field within the i-layer. This results in a decrease of the electron-hole collection at the terminals of the device and can be interpreted as a change in the voltage-dependent quantum efficiency. The described behaviour is responsible for the voltage dependent photo-current in a-Si:H solar cells, which was part of the discussion in chapter 2. Additionally, it is shown that there are two effects determining \( EQE-V \) characteristics, the first is that the observed decrease of \( EQE \) is more significant for thicker i-layer cells. The second is the degraded devices have shown stronger decreases in terms of the voltage-dependent \( EQE \). The reasons causing this behaviour have been identified in the end of section 4.2 and therefore, will not be reproduced here. One should note though, that the results shown here are in agreement with the observations of others scientists such as Yang et al. [110] and Hack et al. [63], as the \( EQE \) of the thinnest device is less sensitive to voltage increases, as well as the \( EQE \) of devices in the as-prepared state.

These considerations remain qualitative and therefore cannot fully explain the deviations shown for high and low APE spectra in previous sections. In order to do this,
the change of the chromatic dispersion of a-Si:H devices with voltage are also examined, as this will determine the magnitude of changes in the PV performance evaluation of a-Si:H solar cells.

Figure 57: Simulated $EQE$-$V$ characteristics for the a-Si:H solar cells of i-layer thickness 250nm (a), 400nm (b) and 600nm (c) in as-prepared and degraded state. The EQE characteristics correspond from increasing voltages from short-circuit to open-circuit conditions.

The partial collection efficiency, $q$, has previously been defined as a useful quantity for investigating the behaviour of the voltage-dependent $EQE$ of a-Si devices ([29], [62])
and is used here for the same purpose. The partial collection efficiency is essentially the $EQE$ of a device under an applied voltage $V$, normalised by its $EQE$ at $-1V$, as given by the following formula:

$$q(V, \lambda) = \frac{EQE(V, \lambda)}{EQE(-1V, \lambda)}$$

(87)

By substituting in formula (87) the computed $EQE$ characteristics for different i-layer thicknesses and level of degradation, one can calculate $q$ in respect to applied bias.

In Figure 58 it is shown that the $EQE$ characteristics of all devices exhibit a decrease with increasing applying bias. As noted before, the observed decreases are stronger with increased i-layer thickness and level of degradation. However, the decrease is not symmetric and differs strongly with wavelength and device state. The later is the main reason different a-Si:H devices show dissimilar performance with spectral variation. It is shown that wavelengths in the red, infra-red region (650-800nm) are prone to stronger quantum efficiency changes with increasing bias. In contrast wavelengths in the blue-green spectral region (380-550nm) are less affected to changes with voltage in terms of $EQE$, which is shown by the plateau $q$ displays in this region. The existence of plateau reveals there is a symmetric decrease in the $EQE$ characteristics, but also there would be no significant deviation of performance in this region providing all devices have been calibrated to produce the same $J_{SC}$. In view of this it can be understood, why the device performance variation also a showed plateau for the case of monochromatic excitation in the blue region (Figure 54).

The results displayed in Figure 58 also reveal that the green-orange spectral region (550-650nm) shows the highest $q$. The superiority of this spectral region in terms of $q$ becomes even more noticeable with increased applied voltage. The physical meaning of the above mentioned behaviour is that photons with wavelength lying between 550-650nm are most beneficial for device performance, as they enjoy high collection efficiency from short circuit to open circuit conditions and as a result will have the highest $FF$. Therefore, the peaks of $J_{SC}$, maximum power output and $V_{OC}$ observed in Figure 54 and Figure 55, can also be attributed to this behaviour, as they are located in the same spectral region. It is also the reason in the spectral region with APE 2.16-2.07eV (575-600nm), where the majority of outdoor spectral variations occur, blue
shifts are beneficial for the $FF$. An effect, which as already stated, has been recorded by Rüther et al. [108], Gottschalg el al. [114] and Minemoto et al. [118]. A more careful observation of Figure 58 can also reveal that the peak of $q$ is progressively located towards “bluer” wavelengths with increasing operation voltages yielding a shift of the $EQE-V$ peaks towards shorter wavelengths. The latter is also in agreement with the results published Bruns [119], who studied the variations of $EQE$ of a-Si:H devices with applied voltage.

Figure 58: Simulated voltage dependent partial collection efficiency ($q$-$V$) characteristics for the a-Si:H solar cells of i-layer thickness 250nm, 400nm and 600nm in as-prepared and degraded state. The $q$-$V$ characteristics correspond from increasing voltages from short-circuit to open-circuit conditions.
4.7. Spectral Correction Factor

In the above sections the spectral variation of the illumination sources in relation to STC spectrum and its impact on performance assessment of a-Si:H solar cells was investigated. It was also shown that the effects were attributed to the voltage dependence of the quantum efficiency and that different light sources will result in a different evaluation of the performance of a-Si:H devices. What has not been investigated yet are the methods which could be applied to correct the measured deviations arising from the spectral variation of the illumination sources. The latter will be the topic of the discussion in this section.

The spectral mismatch factor, \( M \), is a concept, which allows the correction of \( J-V \) characteristics of test cells taking into account spectral deviations. \( M \) is formulated to correct the observed differences between test and standard spectrum at short circuit conditions. This is essentially achieved by correcting the short circuit current of a device to what it should be at the reference spectrum. It is typically given as [120].

\[
M = \frac{\int_{\lambda_1}^{\lambda_2} E_s(\lambda)S_t(\lambda) d\lambda \cdot \int_{\lambda_1}^{\lambda_2} E_{ref}(\lambda)S_r(\lambda) d\lambda}{\int_{\lambda_1}^{\lambda_2} E_s(\lambda)S_s(\lambda) d\lambda \cdot \int_{\lambda_1}^{\lambda_2} E_{ref}(\lambda)S_s(\lambda) d\lambda} \quad (88)
\]

Dividing the measured photocurrent by the spectral mismatch correction factor reduces the deviation in the photocurrent when measuring a solar cell under a light source \( E_s(\lambda) \) in respect to a reference spectrum \( E_{ref}(\lambda) \). The integration limits \( \lambda_1 \) and \( \lambda_2 \) should be the same for all integrals and are limited by the responsivity ranges of the test cell \( S_t(\lambda) \) and the reference cell \( S_r(\lambda) \), which in the case of a-Si:H solar cells varies between 380nm and 800nm. Nevertheless, the principle of superposition for a-Si:H cell behaviour does not hold, i.e. the quantum efficiency of the device is strongly voltage dependent. Therefore, one cannot assume that applying corrections at short-circuit conditions is an adequate measurement method, as the response of the device will also vary with increasing operation voltage. It is shown that even a perfect calibration of an a-Si:H device at 0V will require further voltage-dependent corrections to eliminate the bias arising deviations.
The impact of different light sources under different forward bias conditions on the spectral correction factor $M$ is investigated here for the same a-Si:H cells examined in the previous sections. In order to do so, the responsivity of the device at 0V bias is assumed to be the “reference cell”, and its spectral response under different forward bias conditions the “test cells” probing propagation of deviations in the performance. Using the expression (88) with the illumination spectra shown in Figure 49, and the calculated voltage-dependent responsivity, one can estimate the voltage-dependent spectral mismatch factor $M$.

The results of the calculations are shown in Figure 59 for the case of the 250nm, 400nm and 600nm i-layer cell in the as prepared and degraded state. It is shown that the
deviation heavily depends on the solar simulator light source, the applied bias and the device state. Therefore, an accurate measurement of the $J$-$V$ characteristics of a device would firstly require the knowledge of its voltage-dependent $EQE$ and secondly the application of the necessary corrections. However, measuring the voltage dependent $EQE$ of a device is impractical, as it requires hardware, which is not available in all laboratories. Therefore spectral deviations of the light sources used for the evaluation of the photovoltaic performance of the device should carefully be selected to approach as possible the standard terrestrial radiation [56].

Sources which deviate strongly to standard terrestrial AM1.5G radiation, require additional corrections, which are not negligible even for a perfect calibration at short-circuit conditions. Although there are minimal deviations for all light sources up to 60% of $V_{OC}$, the deviations are gradually increasing to deviate strongly and become noticeable above 80% of the $V_{OC}$, even for class A solar simulators. This is typically in the region of the maximum power point and therefore has a particular importance for the evaluation of PV performance of a-Si:H devices. For reasons which have been already outlined in previous sections, the mismatch factor deviation also becomes stronger with increasing i-layer thickness and degradation, regardless the light source. Hence, additional care should be taken when measuring heavily degraded devices or devices with increased i-layer thickness with spectra, which do not comply with IEC 60904-3 regulations [56].

An additional point of interest is the behaviour of the 600nm i-layer cell in the degraded state under the illumination of the Tungsten light source and the red LED. In this case the spectral correction factor crosses at 90% of $V_{OC}$ showing a co-variance of the performance deviation to STC of both spectrum and voltage bias. These two light sources are able to cause a maximum underperformance of the device each at a different voltage range. The red LED may cause higher maximum deviations, however it shows smaller deviation to performance under STC conditions from 0% to 90% of $V_{OC}$ for the 600nm i-layer cell. The effect is better illustrated by comparing the relative difference of the $J$-$V$ characteristics of the two sources.

Figure 60 displays that there are indeed two areas, one where the red LED produces lower current density (higher photocurrent response) ranging from 0% to 90% of $V_{OC}$
and a second between 90% of $V_{OC}$ and $V_{OC}$, where the Tungsten light source produces higher photocurrent. This may seem in contrast with the other results presented, which showed a consistent behaviour of performance deviation to different light sources, but can be explained.

![Graph showing the relative difference $\Delta J = J_{\text{Tungsten}} - J_{\text{Red LED}}$ of the simulated current densities simulated for the 600nm i-layer cell in the degraded state corresponding to Tungsten and red LED illumination, as a function of the voltage normalised by its $V_{OC}$ value under STC.](image)

The illumination spectrum of Tungsten (Figure 49) extends to far “redder” and “bluer” spectral areas than the red LED, whose spectrum lies in the narrow circumference of 640nm. It is also shown in Figure 57 and Figure 58 that in general $EQE$ drops appear more severe for “redder” areas of the spectrum ($\lambda > 600\text{nm}$). As applied voltage increases $EQE$ drops progressively increase and become gradually significant for the whole spectrum range, but the highest underperformance is always observed for the lowest energy photons. Photons of wavelength 640nm, which predominantly compose the red LED excitation source, appear to be less affected by $EQE$ changes than photons of wavelength longer than 700nm. Furthermore, photons of wavelength shorter than 600nm, which almost explicitly belong to the Tungsten source, show even smaller $EQE$ changes with increasing voltage. These effects are mainly due to the fact lower energy photons are absorbed deeper in the i-layer than photons of higher energy. This is essentially limiting performance, as holes, which are the low mobility carriers, will have to cover a longer distance in order to be successfully collected at the p-layer. The whole effect is further stressed by increasing voltage, which is limiting the collection of carriers.
Increases of the applied voltage will firstly effect the redder parts ($\lambda>700\text{nm}$) of the spectrum, viewed by the lowest received values of $M$ for the Tungsten light source than the red LED from 0% to 90% of $V_{OC}$ (as shown in Figure 59, f and Figure 60). With further voltage increases, photons of 640nm wavelength will also start to suffer from a reduced $EQE$ resulting in a significant decrease of $M$ corresponding to the red LED light source. This is indeed the case, as at 70% of $V_{OC}$ the slope of $\Delta J$ (Figure 60) becomes negative indicating the effect becomes considerable. At 90% of $V_{OC}$, $M$ equals for both Tungsten and the red LED light sources, as the produced photocurrent is the same for both excitation sources for the second time again. For even higher voltages (>90% of $V_{OC}$) the red LED has significantly lesser $M$ than the Tungsten light source (Figure 59, f). The later is due to the fact the Tungsten light source is also composed of photons of higher energy ($\lambda<600\text{nm}$) than the spectrum of the red LED. The former, as noted before, appear to be less affected by voltage increases essentially balancing the poor collection of low energy photons ($\lambda>700\text{nm}$) of the Tungsten light source. This is due to the fact photons of higher energy are more likely to be absorbed closer to the p-i interface. As a result the average collection path of holes, which have lower mobility and thus restricting device performance, will be shorter enhancing device performance. The described effect requires a strong $EQE(V,\lambda)$ change to become noticeable, which occurs only for the case of the 600nm i-layer cell in the degraded state.

4.8. Conclusions

An issue for the a-Si:H device characterization is the variation of the solar simulator spectrum to the standard terrestrial AM1.5G spectrum. It is shown that different light sources result in deviations in the performance evaluation of a-Si:H solar cells. These deviations are usually small for class A solar simulators, but may be significant for Halogen or LED sources. The magnitude of the deviations arising in the performance evaluation though, does not solely depend on the spectral mismatch between the solar simulator spectrum and the standard terrestrial AM1.5G spectrum, but also the state of the device itself.

The performance deviations have been attributed to the voltage dependence of the quantum efficiency, which affects different wavelengths differently. This means in
practical terms that one should not test a-Si in the production with the commonly used red LED flasher. It was also shown that the device state affects the magnitude of these spectral effects, as deviations seem to be dependent on the level of degradation, but also the i-layer thickness of the a-Si:H device. This voltage dependence of the spectral response implies that the mismatch correction should be carried out on a point by point basis. This would then also remove the need for a ‘calibration’ of the solar simulator which will only work for a very narrow range of devices and actually might result in increased uncertainty in test houses, where the device parameters are not known. This, however, requires the knowledge of the voltage dependent spectral response of a test device, which is not a simple task to measure, together with the knowledge of the time resolved spectrum in the solar simulator, which is also hard to quantify accurately.

Last, it should be emphasised that the accuracy of the performance evaluation of a-Si:H solar cells is very much dependent on the solar simulator illumination spectrum. Therefore, solar simulator spectra should resemble as much as possible the standard terrestrial AM1.5G spectrum in the whole spectral region. Once a significant spectral deviation exists, the impact on the performance evaluation is not negligible. Furthermore, the exhibited deviations cannot be accurately corrected only by a simplified calibration of J-V characteristics at short-circuit conditions. In these cases additional care should be taken, especially when measuring heavily degraded devices or devices with increased i-layer thickness, as the voltage-dependent correction of the spectral mismatch should be employed.
Chapter 5 – Effects of Spectral Irradiance Variation on Outdoor Performance

5.1. Introduction

In the previous chapter, it was shown that the efficiency of the device is greatly influenced by the spectral variations of the excitation spectra. In a similar manner the complex nature of earth’s atmosphere will cause a strong disparity of the outdoor illumination conditions resulting in a deviation of the a-Si:H solar cell efficiencies. As discussed in the introduction of this thesis, the irradiance will not only vary according to the geographic location of the site (Chapter 1, Figure 3), but also with daily, annual and weather-based patterns. It is also known that high irradiances would cause a raise in the module temperature to increase well beyond the STC value. In addition the solar angle of incidence changes on a daily and annual basis and is rarely normal to the plane of the array, which is one requirement defined for STC. To further broaden the irradiance variability, the solar spectrum also is affected by solar position, as bulk attenuation in the atmosphere is wavelength-dependent and the solar beam path length changes with solar elevation. Last but not least, there is an extra dependence on the weather as cloud cover acts to further skew the spectrum.

In order to quantify and study the solar cell performance changes two different methods have been suggested to characterise the output of PV systems under wide-ranging operational conditions. The first is the performance ratio, which is given by the efficiency of the PV module in a period of time over the efficiency of the same module under STCs [16]. The second is the energy yield, defined as the actual electrical energy generated by the system in a given period of time [17].

The aim of this chapter is to examine the correlation of solar cells of different i-layer thickness in different degradation states with the varying incident spectra of outdoor operation. An indication that spectral irradiance changes will impact on a-Si:H solar cell performance has already been given in chapter 4, where it was shown that in several
cases for amorphous silicon solar cells, not always the highest $FF$ corresponded to the highest power output, as spectral changes greatly influenced the $FF$ and the maximum power output. Therefore, the highest power rating of a solar cell may not necessarily correspond to the highest energy yield. Consequently, pricing PV modules on the basis of their power rating may be suboptimal for electricity consumers and suppliers, who buy and sell in units of energy.

The actual energy yield is the key feature. The performance of amorphous silicon solar cells should be investigated in the frame of realistic spectral irradiance changes which occur outdoors. In order to understand the magnitude of performance variations due to outdoor spectral variations, it is imperative to isolate various effects, which may also have an effect on performance. Spectral and non-spectral effects, i.e. shading, temperature changes or the angle of incidence distribution of the incoming light, need to be separated to fully understand outdoor operation. It is not easy to experimentally isolate spectral effects in the outdoor environment, as there is a constellation of independent parameters, which has also a co-variance on performance.

The effect of varying outdoor spectral conditions on the performance of hydrogenated amorphous silicon (a-Si:H) thin-film solar cells has been investigated experimentally by Betts et al. [113], Ruether et al. [108], Gottschalg et al. [121] and Minemoto et al. [118]. The average photon energy (APE) was identified as a useful classification with regard to a-Si:H performance. Ruether et al. [108], Gottschalg et al. [121] and Minemoto et al. [118] base their investigation on outdoor measurements, which de facto inherent a co-dependent on secondary factors, such as temperature, or shading. Betts et al. [113] have suggested a method to model the behaviour of short circuit current density ($J_{SC}$) for a-Si:H solar cells taking into account temperature calibrations. Since though, the spectral response of the device is voltage-dependent (as shown in section 4.6), the performance of the device at maximum power output conditions, may differ from short circuit conditions.

The investigation carried out in this work is based on opto-electrical modelling of devices, as presented in chapters 2 and 3. It allows an understanding of the behaviour of the device in varied spectral conditions without co-dependencies from secondary effects, such as the angle of incidence, or the module temperature.
In this work, a modelling approach is followed to simulate the behaviour of a-Si:H solar cells under realistic spectra. Specifically, the variations of a-Si:H solar cell performance were modelled under spectral conditions measured in Loughborough over an uninterrupted period of one year. Cells of different i-layer thickness and degradation state were probed. The spectral data are investigated in terms of APE and intensity, and are used to simulate the $J-V$ characteristics of a-Si:H solar cells over a broad range of conditions. The continuity of the acquired data ensures that an investigation of the seasonal dependence of performance would also be possible.

The results show there is a seasonal effect on performance which strongly depends on device structure. Finally, the behaviour of the cells under different cloudiness is examined over a range of spectral irradiance data with varying clearness index. Interestingly in both cases, seasonal spectral and clearness variation, it is shown that not necessarily the highest FF conditions result in the maximum power output. The later is indeed essential, as it points out that the highest power rating, may not always agree with the highest energy yield.
5.2. Measurement System and Data Collection

![Figure 61: Rooftop Side of the CREST Outdoor Measurement System in 2003. The system is located at Loughborough (latitude 52°), UK.](image)

The CREST (Centre for Renewable Energy Systems and Technology) rooftop-mounted PV module monitoring system (COMS) was originally commissioned in May 1998 [123]. The system was designed to investigate the performance of the module operating under a broad range of naturally varying environmental conditions. The system is able to simultaneously track the performance of PV modules and collect environmental data on a real-time basis. The outdoor measurement system, which was used to record spectra is described briefly in this section.

The measurements are taken as part of CREST’s performance monitoring [122] and only details pertinent to this work are reviewed here. The collection of the data used for this work occurred in the period of October 2003 to September 2004. At this stage the system was monitoring the outdoor spectral irradiance using a spectroradiometer; a scanning monochromator type with a silicon detector to measure solar spectral irradiance from 300 to 1040nm and a second indium-gallium-arsenide (InGaAs) detector to extend the range to 1700nm. Measurements were taken in 10nm steps, requiring 141 individual samples per scan. The latter in combination with the detector
The switchover period and scan speed leads to a complete spectrum measurement time of approximately 2 minutes, which was carried out in 10 min intervals from dawn to dusk.

A possible source of errors may arise from changing sky conditions during the scan time. In the cases where the change is excessive, the data are not considered in this thesis. The tolerance was set to 5% irradiance variation. Such kind of variations may skew the actual measured spectrum, but since a change in either direction, it is unlikely that a statistically significant bias has been introduced.

Additionally, the measurement system experienced some minor faults. Primarily this relates to timing mismatch errors, where it has often been ambiguous whether or not the data file timestamps have been adjusted for local daylight saving and other problems relating to the system clock. These issues occurred mainly during the summer of 2004, and especially in June 2004. Consequently, the volume of the spectral data during this period is reduced.

5.3. Characterisation Methods of Outdoor Illumination Conditions

5.3.1. Spectral Characterisation

Ideally, a spectral distribution would be summarised as a single parameter, which could then be used in much the same way as broadband irradiance, or the device temperature to isolate and quantify the different environmental effects acting the PV device. In practice, this is not easily achievable, as spectral irradiance data consist of an ensemble of measurements, which does not lend itself well to use in simple analysis or modelling approaches. For this reason, several approaches have been suggested to characterise the spectral irradiance.

The colour temperature is a fundamental method of characterising spectra, which is associated with the temperature of a blackbody radiator. This method may be well sufficient to represent the solar spectrum outside the Earth’s atmosphere, but is
unsuitable for terrestrial application [17], because the various gas absorption bands and wavelength dependent scattering prove too distorting.

One of the most established methods of spectral characterisation is the calibration number, $CN$, as suggested by NREL [124]. The CN is based on the variation of the short-circuit current of a photovoltaic device against the broadband irradiance.

$$CN = A \frac{\int_{\lambda_{min}}^{\lambda_{max}} E_i(\lambda) \cdot SR(\lambda) d\lambda}{\int_{\lambda_{min}}^{\lambda_{max}} E_i(\lambda) d\lambda} = \frac{I_{sc}}{G} \quad (89)$$

It should be noted; that $G$ here represents the total broadband irradiance within integration limits $\lambda_{min}$ and $\lambda_{max}$ and should not be confused with the generation rate of the device. $A$ is the active cell area, $E_i$, the spectral irradiance corresponding to wavelength $\lambda$ and $SR$ is the wavelength-dependent spectral response of the examined device. For ideal spectra $CN$ should equal the fraction of $I_{sc}/G$ under standard test conditions. The main drawback of this method is its device-dependence, as formula (29) is a function of the spectral response of the device.

This chapter aims to be device independent. For this purpose $CN$ is not adequate, as it cannot provide a comparison bases for illumination spectra, which excite amorphous silicon solar cells of varied i-layer thickness and degradation states, since the spectral response of these devices will be different. Therefore, the investigation carried out here is obliged to be restricted on device-independent methods of spectral characterisation.

Such method of characterising spectra is through the use of the average photon energy ($APE$), as defined by Betts et al. [113]. The $APE$ is a device-independent spectral descriptor, which allows the characterisation of spectra with a single number; making it attractive for processing a large number of spectra. In view of the fact that this work focuses solely on amorphous silicon solar cells, $APE$ here refers to the average photon energy of photons in the active photovoltaic spectra area of a-Si:H solar cells, which is 380-800nm. The later is done, because taking into account in the spectral weight photons which as shown in chapters 2 and 3 do not contribute to electrical collection, may result in misleading judgements on performance. Studying spectra with their $APE$
may lose resolution and may not reflect all features seen in outdoor conditions, but allows a flexible characterisation of every spectrum with a single number.

The $APE$ of a spectrum nonetheless, does not contain information on the broadband irradiance of a spectrum. Thus, the recorded spectra will also need to be examined in view of their corresponding broadband irradiance, $G$. In this case, $G$ also refers to the broadband irradiance in the spectral area of 380-800nm and corresponds to 555.38W/m$^2$. Generally, the performance parameters of the cells, $J_{SC}$, $V_{OC}$, maximum power output and the $FF$, are examined against the corresponding irradiance in the window of 380-800nm. For the case of efficiency calculation though, the total broadband irradiance (300-1700nm) is taken into account, unless specifically stated.

5.3.2. **Sky Clearness Characterisation**

The opacity of the atmosphere is generally represented by the clearness index, $k_T$, defined as the ratio of total irradiance measured on a horizontal plane at the Earth’s surface, $G_H$, to the total extra-terrestrial irradiance incident on a horizontal plane at the top of the atmosphere [17]:

$$k_T = \frac{G_H}{G_0/AM}$$  \hspace{1cm} (90)

where $G_0$ is the solar constant and $AM$ the air mass. However, this parameter is not independent of the air mass since it is a measure of the total broadband attenuation and hence is affected not only by the amount of cloud present, but also by the atmospheric path length. Generally, cloudy conditions correspond to low clearness index (smaller than 0.6), while clear sky conditions may have clear index values, which approach unity (approximately in the range of the $AM$).
5.4. Effects of Angle of Incidence on performance

This chapter focuses on the effects of outdoor spectra on a-Si:H solar cell performance. Therefore, it is important to eliminate any side effects on performance arising from the variation of angle of incidence, $AoI$, of the illumination conditions. Specifically, identical spectra will cause a different a-Si:H solar cell performance, when the $AoI$ of the incoming photon flux do not match. As a consequence, the effects of the $AoI$ on performance should be taken into account, when comparing any spectra. Ideally, the investigated spectra should all correspond to the same angle of incidence, in order to provide a consistent set of studying conditions.

![Diagram](image)

Figure 62: Graphic description of the angle of incidence, $\theta$, in relation to the plain of the array (PoA) and the position of the Sun.

However, in the continuously changing outdoor conditions, the latter is not a realistic objective. Hence, the impact of varying $AoI$ illumination conditions on the performance of a-Si:H solar cells should be investigated. The goal here is to seek a range of $AoI$ conditions, where the performance of a-Si:H solar cells does not deviate significantly. Thus, under such a frame of conditions the direct comparison of measured outdoor spectra would be valid without significant secondary effects arising from changes of the $AoI$. 
The angle of incidence, $\theta$, for an inclined plane is described as the angle between the centre of the solar disc and a point on an irradiated surface and the outward normal to the irradiated surface, as shown in Figure 62. The effect of angle of incidence on the performance of PV devices is the result of two main effects. Firstly, the ‘cosine effect’ related to the geometrical factor (cosine law) [125], which basically limits the transmission of oblique angles within the device. Secondly, the ‘optical effect’ related to the reflection of light at more oblique angles and the disparity of light confinement within the device, which appears to be different under normal and oblique angle of incidence [126].

Figure 63: The relationship between the normalised short circuit current, $I_{SC}$, and the normalised plane of array irradiance, $G_{PoA}$, for amorphous silicon module measured at CREST in clear and cloudy sky conditions including reflectance angular dependence [127]. The theoretical linear dependence of an ideal cell is shown as a straight line and the point for 50° is indicated.

The effect of angle of incidence of the main solar beam on a-Si:H performance in correlation with the short circuit, $I_{SC}$, current and the broadband irradiance at the plane of the array, $G_{PoA}$, was experimentally studied by Williams et al. [127]. Figure 63 shows the relationship between ISC and GPOA of a single diode a-Si:H PV device under varied spectral conditions in relationship to changes of AoI and cloudiness. The straight line indicates the ideal relationship, where the calibration number, $CN$, would remain constant to its value under STC regardless the spectral variation. The dots correspond to measurements taken under clear skies, while the crosses under cloudy sky conditions. It can be seen that for small angles of incidence the device follows closely the ideal behaviour, which seems to be a fair approximation up to 50° of AoI.
Departures from the ideal behaviour start to occur for angles greater than 50°, which is an indication that the effects of the angle of incidence becomes considerable.

Therefore, increased incident angle \((AoI > 50°)\) may introduce non-negligible secondary effects on a-Si:H solar cell performance. Attributing these effects to spectral variation would be erroneous, as it was shown in Figure 63 there is also a correlation of \(AoI\) and performance. Thus, a correct examination of spectral effects on performance would require an elimination of such conditions. For this reason, only the spectra which correspond to angles of incidence smaller than 15° will be included in this work. The angle of incidence limit was selected, because the effect seems to be negligible in this range \((AoI < 15°)\), but also because the remaining spectra are sufficient in quantity (one thousand) to statistically reduce any errors arising from experimentation. The selected spectra and their properties is the subject of the discussion of the next section.

5.5. Outdoor Variation of Spectral Irradiance

The current section presents the spectral irradiance measurements, which will be used to investigate the effects of spectral variation on performance. All the measurements were carried out at CREST during the period of October 2003 to September 2004, as described in 5.2. The installation of the PV monitoring system was initially readied by Professor Ralph Gottschalg [123]. Later Dr. Thomas Betts [17] improved the system and collected the measurements which are used as input in this research. There are three thematic subsections here; the first examines the spectra in terms of intensity, \(G\) and \(APE\), the second examines seasonal effects on spectral variation and the third effects of cloudiness on spectral distributions. The main approximation carried out in this work is that the angle of incidence is considered normal to the plane of the array at all cases. This may not be the case for all spectra, as some spectra may correspond to oblique \(AoI\). In this way however, the spectral effects on performance are comparable and are not affected by \(AoI\) effects.
5.5.1. Effect of G and APE on the Measured Outdoor Spectra

![Figure 64: The distribution of the measured spectra in relation to their irradiance, G, and APE is shown for two cases (a) broadband spectrum (300-1700nm) and (b) PV effect spectral region of a-Si:H solar cells (380-800nm). The data group which corresponds to clear skies and high solar elevation is marked as I, while the data group corresponding to cloudy conditions as II. The area, which corresponds to STC is indicated with a red dot.](image)

The measured spectra are displayed in respect to their calculated irradiance, G, and APE distributions in Figure 64. The spectral data are filtered to satisfy a maximum AoI condition of $\theta < 15^\circ$, for the reasons discussed in section 5.3. The remaining spectra are characterised using the methods examined in 5.4.

An observation of Figure 64 shows that the illumination conditions varied significantly during the time period of October 2003 to September 2004. It is also shown that there are two main data groups, which seem to be discrete and attract the majority of spectral data. The first group, which is marked as I in the graph, corresponds to clear skies and high solar elevation, and shows predominantly high irradiances. The second, which is marked as II, is compiled of spectral data of lower irradiance and corresponds to conditions of increased cloudiness. It should be noted that low irradiances can be caused either by clouds or by high air mass. In this case, the data group II is dominated by clouds, because by filtering the spectral data to $\theta < 15^\circ$ essentially also filters the data corresponding to air mass higher than ~2.5. Additionally, during the quality check, which is applied in the measurement time, an amount of data is filtered out. Data with intensities in the area of 500W/m² are often filtered out, when they correspond to unstable irradiance conditions (such patchy clouds, which are dynamically changing). As a result the distribution between clear and cloudy data is further stressed.
Another point of interest in Figure 64 is the impact of $APE$ on the recorded spectra. It is observed that there is a clear correlation between $APE$ and the two discrete data groups. Specifically, data group I, shows a lower $APE$ on average than group II. The effect is attributed to the impact of cloudiness, which it is known to act as a high-pass filter and limit low energy photons [17]. As a consequence, the data group I, which corresponds to clear sky conditions, has on average a lower $APE$ than the data group II.

The spectral data shown in Figure 64 are investigated in terms of both broadband spectrum (300-1700nm) and the PV effect spectral window in a-Si:H solar cells (380-800nm). The latter is examined, because not all photons which reach the i-layer will contribute to photo-generation and eventually successful electron-hole collection at the terminals of the device. As shown in chapter 2, high energy photons ($\lambda<380$ nm) are screened either by the TCO or the glass, while low energy photons ($\lambda>800$ nm) do not contain sufficient energy to cause photo-excitation. Therefore, it may appear misleading to take into account in the calculations of performance variations of a-Si:H in terms of $APE$ and $G$, photons which de facto do not contribute to the electron-hole collection. It should be noted that when restricting the spectrum to 380-800nm, there seems to be a linear correlation between $APE$ and $G$, which is not visible when examining the whole spectrum.

Another observation from Figure 64 is that only a very small part of the recorded spectra matches the STC (indicated in Figure 64 with a red dot). It is shown that the STC correspond only to a narrow area of the actual outdoor operating conditions, close to the far edge of high intensity conditions. In addition, the recorded spectral irradiance changes clearly occur towards both $G$ and $APE$, simultaneously. As it was shown in the previous chapter, both will affect the efficiency of the cell independently. Therefore, rating the cells using the STC efficiency as a benchmark is insufficient to describe holistically the effects, because different spectral irradiance conditions may correspond to the same power rating. A detailed investigation of power rating variation is given in a following section.
5.5.2. Seasonal variation of the measured spectral distributions

The seasonal changes of the recorded spectra are the subject of the discussion in this subsection. Spectral effects are examined here in terms of monthly averages, which reduce the quantity of the data and allow an easier and direct comparison of the measured spectra. It should be noted that the spectra examined in this section are not filtered by AoI criteria. This is due to two practical reasons; the first is the reduced volume of data in June 2004, which was the product of faults in the measurement system. The second is that limiting the AoI also reduces the volume of measurements taken in December, as the main solar beam reaches its maximum obliqueness during this month [127].

![Seasonal Spectral Variation](image)

Figure 65: Normalised monthly average measured spectral irradiance against wavelength. The spectral weight is shifted from shorter wavelengths to longer wavelengths moving from summer to winter months.

The monthly averages presented here are the average spectral recordings from dawn to dusk and therefore any side-effects arising from AoI variation should affect all spectra. Strictly speaking, the winter months are more severely affected by oblique angles of incidence, which is neglected here. As a consequence the results shown here, would underestimate the magnitude of seasonal performance variation favouring the winter months, because for the purpose of the simulations normal incidence is assumed for all spectra. However, as it will be shown in following sections, there is still a significant effect arising solely from the variation of average spectral distribution and intensity, which cannot be neglected.
In Figure 65 the variation of the normalised average monthly spectral distributions is shown. As it can be seen, there is clearly a seasonal effect, which shifts the spectral weight towards longer wavelengths during the winter. This is due to air mass reaching its minimum during summer, and thus spectrum skewing towards blue wavelengths [114]. Figure 66 displays the variation of the average intensity in the 300-1700nm spectral region. As expected the irradiance increases significantly as moving from winter to summer months. The apparent low irradiances displayed here are explained, because recordings include data measured from dawn to dusk, which are then averaged again for every month.

A point which requires attention is the rather odd behaviour recorded during the summer of 2004. This summer has been “poor” even for British standards in terms of average irradiance, as the weather has been predominantly cloudy. This can be seen by the relatively low monthly average intensities, which have been recorded. In any case, the spectral data shown in Figure 65 still demonstrates significant spectral differences between summer and winter, which require investigation. Despite the shortcomings caused by the poor irradiances recorded during the summer of 2004, the set of spectra also point out in the best possible way the chaotic nature of outdoor conditions, which always remain unpredictable.
5.5.3. Effects of sky cloudiness on the measured spectra

As it was earlier stated in 5.3.2, the sky clearness index does not solely depend on sky cloudiness, but also on the air mass. Hence, it expresses the total attenuation, which takes place in the atmosphere. It is known that the air mass varies from winter to summer. Therefore, in order to examine the effects of cloudiness on performance, it is required to isolate effects arising from the variation of air mass during the year.

For this study, six different spectra, all recorded in June 2004, between 11:40 and 12:20 at noon, exhibiting different sky clearness indices were selected. It is important to mention, all spectra were measured around noon time in June, when air mass reaches its minimum. As a result all spectra correspond to sky conditions with similar air mass. Additionally, there are no significant effects due to the variation of AoI, as at all cases the AoI is below 10°.

The selected spectra are plotted in Figure 67. The clearness index, $k_T$, of the selected spectra is shown within brackets. The spectral red-shift observed from cloudy to sunny weather conditions is highlighted.

For this study, six different spectra, all recorded in June 2004, between 11:40 and 12:20 at noon, exhibiting different sky clearness indices were selected. It is important to mention, all spectra were measured around noon time in June, when air mass reaches its minimum. As a result all spectra correspond to sky conditions with similar air mass. Additionally, there are no significant effects due to the variation of AoI, as at all cases the AoI is below 10°.

The selected spectra are plotted in Figure 67. The clearness index is issued here to characterise the cloudiness of the sky conditions. As discussed in section 5.3.1, it is shown that clouds act as a high band-pass filter and limit low energy photons. Consequently, the spectrum is skewed towards bluer spectra for increased cloudiness conditions (low clearness index). It should be noted that the case of $k_T > 1$ is not unphysical, but corresponds to a case where the diffuse irradiance in the measurement location is higher than the attenuation of the beam component in the atmosphere.
5.6. Effects of Irradiance Spectrum on Performance

In this section the outdoor spectra measured and characterised in section 5.5 are used to simulate the performance of a-Si:H solar cells. The a-Si:H solar cells examined here are the same which were used in the investigation carried out in chapter 4. Specifically, three cells of i-layer thickness 250, 400, 600nm under two degradation states (as-prepared and degraded) have been selected, because both factors have a significant effect on device performance. These i-layer thicknesses represents the typical range of a-Si:H commercial devices [27]. The influences of both i-layer thickness and degradation on performance are also co-dependent on the illumination conditions, as detailed in section 4.2. It is shown that indeed these two factors have an impact on performance, the magnitude of which varies with spectral changes observed at the outdoor environment.

5.6.1. Effects of Intensity on performance

The simulated performance characteristics ($J_{SC}$, $V_{OC}$, $FF$, Maximum Power Output) of the cells detailed in section 4.2 are investigated here. The percentage variation of $J_{SC}$ and maximum power output to STC values is given in Figure 68. The graphs presented here, should ideally contain two fixed points. The first point should have coordinates ($G_{STC}$, 0), corresponding to STC intensity, which is ~550 W/m$^2$ in the 380-800nm spectral region. The second point should have coordinates (0, 100), for zero photon influx conditions. The ideal relationship would impose a linear relationship of intensity, $G$, and the short circuit current $J_{SC}$.

For this investigation, intensity is limited between 380-800nm, which is the active region of the PV effect in a-Si:H solar cells. Both power output, and especially short-circuit current density ($J_{SC}$) have a linear behaviour. One should note the observed linearity is due to the fact the APE of outdoor spectra did not change significantly (Figure 64). Maximum APE change hardly exceeded 0.1eV in the 380-800nm region. Our simulations had shown (Chapter 4, Figure 55) that when the APE changes more noticeably >0.2eV, the power output seem to be affected by non-linearities. Nevertheless, this is not the case for outdoor spectral variations, which seem to be less
prone to non-linear effects. This may be a good first order approximation in all cases, which seems to hold not only for $J_{SC}$, but also for maximum power output.

Non-linear effects though, should not be ignored. A more careful observation of the graphs reveals the existence of second order non-linear effects. Firstly, the linear fittings shown in Figure 68 are not identical. There are deviations, which become larger for increased i-layer thickness and level of degradation. Secondly, there is a repeated pattern in all graphs (as shown in Figure 69). This shows that the percent variation is overestimated for low intensities, $G < 300$ [W/m²] (380-800nm) and underestimated for high intensities, $G > 400$ [W/m²] (380-800nm). The magnitude of these deviations is also amplified for increased i-layer thickness and level of degradation. Since all the parameters but the spectrum, are kept constant, these effects cannot be attributed solely to sheer intensity changes.

Figure 68: Variation of the simulated performance parameters of the examined cells with intensity changes in the spectral region of 380-800nm in terms of short-circuit current density and power output for cells of different i-layer thickness (250nm, 400nm and 600nm) and level of degradation (as-prepared and degraded state). The variation is calculated at all cases in respect to the values of the performance parameters under STC.
Figure 69: Deviations to the simulated linear behaviour of $J_{SC}$ and power output variations exhibit in both low (a), $G < 300$ [W/m²] (380-800nm) and high (b), $G > 400$ [W/m²] (380-800nm) irradiance regions, which may arise above 5%.

For the case of open circuit-voltage, $V_{OC}$, an increase with increasing intensity was observed. The increases follow a logarithmic trend. The percent variation of $V_{OC}$ to $V_{OC}$ under STC seems not to be significantly affected by the i-layer thickness of the cells. In most cases the observed differences were almost of the same order of magnitude. The level of degradation though did show an effect increasing the percent differences by approximately 2-3%. In a similar manner with $J_{SC}$, $V_{OC}$ variations follow a specific trend with intensity changes. At the same time fluctuations were observed to conditions which correspond to identical intensities, but did not exceed 0.8% of the percent value.

Figure 70: Variation of the simulated performance parameters of the examined cell with intensity changes in the spectral region of 380-800nm in terms of open-circuit voltage, $V_{OC}$, and the fill factor, $FF$, for cells of different i-layer thickness (250nm, 400nm and 600nm) and level of degradation (as-prepared and degraded state). The variation is calculated at all cases in respect to the values of the performance parameters under STC.
The fill factor (FF) exhibited a reversed U-shape behaviour varying with increasing intensity. The maxima of the described curve extend in light intensities of 90-180 W/m². Under low-irradiances (< 100W/m²) the FF of a-Si:H solar cells seems to be affected by non-linear effects, which hamper the maximum power output (as seen in Figure 69, a) and cause lower performance than expected. However, moderate intensities (> 300W/m²) also cause lower FF, as seen in section 4.5. With these two effects limiting the FF under low and moderate to high intensities, the FF reaches its maximum in the area in between (90-180W/m²). Generally, it is shown that at all cases both increasing i-layer thickness and degradation also increase the magnitude of FF variation.

A case of interest is the 600nm i-layer cell in degraded cell. In this case the FF shows an almost linear behaviour decreasing with increased light intensity. This behaviour is caused due to increased recombination dominating the performance of this cell, but also the magnitude of the electric field, which is weaker for thicker i-layer cells. As a result the curvature of the J-V characteristics is affected significantly at increasing forward voltage. The later is consequently causing an almost linearised variation of the FF with increasing voltage. The described effect is not a numerical error of the simulation. This is shown in Figure 71, where the Merten model has been used to describe the behaviour of a 600nm i-layer device. Although, the equivalent circuit differentiates quantitatively the magnitude of FF deviation, qualitatively shows there is a direct correlation on steepness and the magnitude of the effects on the level of degradation.

![Figure 71: Normalised deviation of the FF with increased light intensity to STC value calculated with the Merten model. It is shown that increased recombination has an effect on the magnitude of the deviation, but also the steepness of the curve with increasing intensity. The modelling parameters used are: \( I_0=1.019 \times 10^7 [\text{mA/cm}^2] \), \( I_{ph}=17.76 [\text{mA/cm}^2] \), \( R_s=1.68 \times 10^{-3} [\text{k}\Omega \text{cm}^2] \), \( R_P=71.88 [\text{k}\Omega \text{cm}^2] \), \( A=2 \), \( V_b=1.1 [\text{V}] \), \( \mu \tau_{eff}=10^{-10} - 10^{-11} [\text{m}^2/\text{V}] \), \( d_i=600 \text{nm} \).]
Another observation is that the $FF$ often varies up to 2% for identical intensities. Since, all the parameters are kept constant, but spectral distribution, it consists a clear indication of secondary effects. Ruether et al. [108] has also examined identical broadband intensities and observed a similar deviation on the value of the $FF$, which was attributed to the spectral changes. Specifically, “bluer” spectra were characterised as beneficial for the $FF$, while “redder” spectra to have a negative influence on the $FF$. Such effects, as well as the impact of spectral distribution on a-Si:H solar performance will be the discussed in the following part.
5.6.2. Effects of APE on performance

It was shown in the previous section that the outdoor intensity variation is responsible for first order effects governing the performance of a-Si:H solar cells, which may vary STC power output from -80% to +10%. At the same time secondary effects were observed, which cannot be solely explained with intensity changes, such effects have been in the order of ±5% of STC power. In this section, it is investigated whether the distribution of the spectrum itself may have an impact on performance of a-Si:H solar cells. For this reason the performance parameters of the cells are investigated in correlation to the APE of the spectra.

The effects of varying APE on the performance parameters in terms of percentage change to performance of the cell under STC, are shown in Figure 72 and Figure 73. For $J_{SC}$, power output, $FF$ and $V_{OC}$ one can clearly distinguish between two APE regions; which were pointed out in 5.5.1. Region I is corresponding to clear skies and
high solar elevation. In this area it is directly observed that increasing APE causes an increase of $J_{SC}$ and maximum power. Under cloudy conditions (region II), the spectrum is blue shifted, but there is no significant correlation to performance. The later could be explained as cloudy conditions have predominantly low irradiances, which can cause a drastic drop at performance. Therefore, the chaotic nature observed at region II is the result of two opposing effects. One is that spectra have higher APE, that is beneficial for performance; the second is that these spectra have often very low irradiance, which has a negative on $J_{SC}$ and maximum power output.

Generally, it can be seen that increasing APE is beneficial for the performance of a-Si:H. Consequently, the variation of APE is identified as a significant factor, that can cause non-negligible secondary effects on a-Si:H solar cell performance. However, as it was shown in chapter 4, not all blue-shifted spectra are beneficial for performance. One should take into account the magnitude of blue shifts, which occur outdoors. At most cases APE varies between 2.10-2.20 eV, which corresponds to average photon wavelength changes from 590 to 560nm. A careful examination of Figure 55 shown in
Chapter 4, shows that in this area blue shifts are indeed beneficial for performance. Therefore, not blindly all blue-shifted spectra are beneficial for performance, but blue-shifts which occur at a realistic outdoor environment are beneficial for performance.

The open-circuit voltage, $V_{OC}$, as shown in Figure 73, seems to be much more susceptible to decreases than increases in relation to $V_{OC}$ under STC. As it has been the case with intensity variation the percent variation of $V_{OC}$ to $V_{OC}$ under STC, seems not to be significantly affected by i-layer thickness of the cells. In most cases the observed differences were almost of the same order of magnitude. In contrast, comparing the as-prepared to the degraded state, shows that the percent variation of the degraded state is higher.

The $FF$ seems to be affected negatively in the region I of clear skies and high irradiance. Nonetheless, these effects are probably caused by high irradiances, which were shown (4.5 and 5.6.1) to have a negative impact on the $FF$. The maximum value of $FF$ is observed in region II of high cloudiness and low irradiances. In this region the $FF$ is showing a marginal increase with increasing $APE$, which almost reaches a plateau after 2.15eV. It should be noted that degradation and increased i-layer thickness consistently augmented the magnitude of $FF$ deviation to STC $FF$, as shown Figure 73. Interestingly, it is also pointed out that the maximum outdoor power output of an a-Si:H solar cell, does not occur under conditions where the $FF$ reaches its maximum. This proves that the $FF$ should not be used as a benchmark to judge solar cell performance.
5.6.3. Effects of seasonal variation on performance

In this section the effects of seasonal variation are investigated. The average monthly spectral irradiances presented in 5.5.2 are used to calculate the electrical behaviour of a-Si:H cells, which were established in 4.2. There are two main seasonal effects, which distort the spectra and cause a variation of solar cell performance. The first is the higher irradiance of the summer months; the second is the blue-shifted spectra recorded for summer months. It is shown that both have a non-negligible effect on performance.

![Graphs of monthly variation of simulated performance parameters for examined cells.](image)

Figure 74: Monthly variation of the simulated performance parameters for the examined cells. The variation is calculated at all cases in respect to the values of the performance parameters under STC.

The results shown in Figure 74 identify that at all cases there has been an underestimation comparing to STC performance parameters. One should take into account that the seasonal variation was investigated on the basis of spectral monthly
averages in terms of intensity and spectrum. Therefore, the exhibited underestimation for all performance parameters is expectable, since at all cases the incident intensity was lower than the STC. In addition the summer of 2004 has been relatively poor in terms of irradiances, which affected mostly June and July. Nevertheless, the irradiances recorded in August, September and October, were considerably higher than all the other months.

The results clearly show that sunnier months, which in this case were August, September and October, delivered the best $J_{SC}$, maximum power yield and $V_{OC}$. This is due to the fact broadband intensity is the dominating factor in PV performance. However, secondary effects arising from the distribution of the spectrum should not be neglected. A good example is the case is February, which has average broadband intensity of 318.8 W/m$^2$, higher than May which has 306.35 W/m$^2$. Despite this difference May shows marginally higher maximum power output than February. This effect is attributed solely to the spectral change, as May spectrum appears blue-shifted comparing to February (Figure 65).

On the contrary to all the other underestimated parameters, the $FF$ is the only parameter which is consistently overestimated. This is due to the fact that $FF$ benefits from moderate intensities (200-500W/m$^2$), typical of the average spectra examined. The latter is also the reason that the $FF$ reaches its minimum overestimation in August, September and October, that have been the brightest months. In addition to high intensities, extremely low intensities as seen in December, seem also to have a negative influence on the $FF$. Months with moderate average intensities, such as February, March or May, benefit the $FF$ most.
5.6.4. Effects of cloudiness of performance

In addition to seasonal variations a number of spectra corresponding to progressively decreasing cloudy conditions (from cloudy to sunny) have been investigated. All spectra were measured in June 2004 at 12 p.m., and correspond to angle of incidence lesser than 10 degrees. For the purpose of simulation an angle of incidence perpendicular to the plane of the array has been assumed.

![Figure 75: Effects of spectra with different clearness index on the performance parameters of a-Si:H solar cells. The simulated performance variation is calculated at all cases in respect to the values of the performance parameters under STC.](image)

The short circuit current density, power output and open circuit voltage, show a steady increase with cloudiness. Despite the increase, the $FF$ reached its highest value at high cloudiness (Figure 75). The highest $FF$ was not simulated for the spectrum with the lowest clearness index, but for the spectrum with the second lowest clearness index. A possible explanation for this is the very low irradiance of the spectrum with the lowest clearness index, not exceeding 144 W/m$^2$. The simulations show that high cloudiness
results in a drastic decrease of performance, mainly $J_{SC}$ and the maximum power output. In contrast, low cloudiness and high intensity conditions, corresponding to high clearness index, do not benefit the $FF$, but yield a high $J_{SC}$ and maximum power output.

The results show the performance of a-Si:H solar cell under cloudiness is primarily driven by the sheer photon influx on the plane of the area of the cells. Secondary effects though, due to blue-shifted spectra caused by cloudiness also exist. Such effects can be seen as the $FF$ reached its maximum value at low clearness index conditions. However, one should also take into account that the reduced light intensities may also cause an increase of the $FF$. The latter is not a reason though, to discard any effects caused by the spectral variation. As it was shown in section 4.5 for the case of monochromatic excitation sources, both effects will occur simultaneously. The simulated changes of the $FF$ are significantly higher in degraded devices, or devices with higher i-layer thickness. These devices seem to be more susceptible to performance variations recording in the simulations the highest overperformance, but also the lowest underperformance. On the other side thinner devices, which are also less prone to degradation effects, seem to have a more stable power output.

5.7. Performance Ratio and Energy Yield

The goal of this section is to review the two main methods which are applied to characterise the performance of solar cells with particular focus to a-Si:H PV applications. The first is the performance ratio $PR$, which is the efficiency of the PV module in a period of time over the efficiency of the same module under STCs [16]. The second is the energy yield, defined as the actual electrical energy generated by the system in a given period of time [17].

So far the effects of various outdoor spectral changes on performance have been investigated. It has been shown that both spectral irradiance and spectral distribution will have an immediate effect on the performance characteristics of a cell. It is crucial to examine the two methods that are being used, and probe whether or not they can reflect the differences between different devices and provide a credible performance.
assessment of them. Since the energy yield of the device is directly proportional to its maximum power output, therefore the maximum power output of a device is reproducing here any changes of the energy yield as well. In the current investigation the PR and the power output is calculated in reference to the performance in the whole spectrum (300-1700nm).

In the first group of graphs (Figure 76) the PR and the maximum power output of the examined devices are plotted against broadband intensity. For the performance ratio there are clearly distinguished two groups of data, one corresponding to high cloudiness (group I) and another corresponding to high irradiances and clear skies (group II). Firstly, the PR seems more susceptible to changes for devices of increased i-layer thickness and level of degradation. The differences may be small but noticeable and are especially shown when comparing extreme cases such as the 250nm i-layer device in the as-prepared state to the 600nm i-layer device in the degraded state. The 600nm i-layer device in the degraded state is the one which underperformed most, as seen by its power output. However, it is also the device which shows the highest and the lower PR. It is shown that the PR of all devices overlap for a very wide range of light intensity

Figure 76: Variation of the simulated performance ratio and maximum power output in respect to broadband intensity for devices of different i-layer thickness and degradation state.

In the first group of graphs (Figure 76) the PR and the maximum power output of the examined devices are plotted against broadband intensity. For the performance ratio there are clearly distinguished two groups of data, one corresponding to high cloudiness (group I) and another corresponding to high irradiances and clear skies (group II). Firstly, the PR seems more susceptible to changes for devices of increased i-layer thickness and level of degradation. The differences may be small but noticeable and are especially shown when comparing extreme cases such as the 250nm i-layer device in the as-prepared state to the 600nm i-layer device in the degraded state. The 600nm i-layer device in the degraded state is the one which underperformed most, as seen by its power output. However, it is also the device which shows the highest and the lower PR. It is shown that the PR of all devices overlap for a very wide range of light intensity
conditions, as the method may not sufficiently differentiate between high and low intensity conditions. What is important here is the fact the PR exhibits its maxima at lower light intensity conditions, which are also conditions of the lowest energy yield. Therefore, the increased PR of such low intensities may be misleading overall and favour devices which are designed for moderate cloudiness conditions.

Figure 77: Variation of the simulated performance ratio and maximum power output in respect to APE for devices of different i-layer thickness and degradation state.

When viewing the two methods in terms of their APE the same two groups of data are still noticeable, especially from the point of view of the maximum power output of the devices. The APE corresponds here only to the PV active spectral region of a-Si:H solar cells (380-800nm). An interesting remark is the linearity, which is displayed by the PR for the clear skies group of data, indicated as I, which shows an almost linear increase of performance with increasing APE. The behaviour though, is rather chaotic for the data which corresponding from moderate to high cloudiness and no effects in terms of the APE can be seen. The latter is important as it is shown that the PR of a device, when examined together with the APE of the excitation spectra can provide a systematic separation of performance characteristics. Such linearity is also observed for the
maximum power output, for group I, but to a lesser degree as the data often present an erratic distribution.

Despite the observed linearity of the data corresponding to clear skies and high irradiance, the PR calculation still overlap under very different conditions of APE. In addition, while the power output shows a clear separation of the performances corresponding to data group I and II, the PR often shows contradicting results, such as high PRs corresponding to poor performances. This may often result to a wrong performance assessment of a device, as the PR of a device may produce unrealistic conclusions. For example a poorly performing device, such as the one with 600nm i-layer thickness in degraded state, may show the highest rating when measured under certain conditions. Of course, if the device is measured over a long period, it would be realised that this device is also showing the lowest PR. The latter though, requires longer test time, which may not always be available. However, the PR is usually used to predict the energy yield of a device in a location, where long-term historic irradiance data are available. Therefore, method will provide a fair estimation of the energy yield, since issues arising from low intensities will be balanced by the large amount of data. In any way, the application of PR is should be always done with care and understanding of the illumination conditions and the state of the device. On the other side the energy yield would be able to identify such faults, as its values directly depend on the power output of the device. The main drawback here, is that the method is not suitable for performance prediction, as the actual power output of the device will remain unknown till measured.

Additionally, the rating of any device, should not be undertaken only in respect to STC. The actual outdoor conditions differ strongly, as a result different devices respond differently in a dynamically changing environment. It is better for all devices to be tested under a series of variable conditions. Finally, what matters most in the end is the sheer energy yield over a year of a device, therefore priority should be given to measuring the actual power output of the device instead of its efficiency variation, when possible.
5.8. Conclusions

In this chapter a comprehensive modelling approach, which is able to examine the variations of a-Si:H solar cell performance under different spectral conditions measured at Loughborough UK, was investigated. Although, similar modelling approaches have been suggested before, this is the first time a detailed opto-electrical model is used to monitor outdoor performance and its key factors, namely intensity and APE. This has importance as experimental studies so far were affected by secondary effects such as angle of incidence, temperature and the degree of shadowing. In this work test devices of different i-layer thickness and degradation state were used to probe over a thousand spectra recorded at Loughborough, UK and the results were compared with the performance of the cell under STC.

It was shown that light intensity is primarily responsible for a-Si:H outdoor performance. Specifically, \( J_{SC} \) and power output seem to be in a linear relationship with light intensity, being a fair approximation at the level of APE variation under outdoor conditions. APE however, seem to have a secondary effect on \( J_{SC} \) and power output, but its impact is more significant at high light intensities –when the device has its maximum energy yield- and therefore, should not be underestimated. The role of APE on performance is not “one-dimensional”, as both high APE and low APE may cause a decrease in performance. However, in the outdoor spectral variations an increase of APE will augment the performance of a-Si:H solar cells. An exception to this observation is the case of very low irradiance (<200W/m²), which often have very high APE, but are strongly unfavourable for performance.

The performance of a-Si:H solar cells is shown to be affected strongly on the spectra as both seasonal variation and cloudiness will skew the spectrum and as a result the \( J-V \) characteristics of the cells. Spectra which have almost the same intensities, may differentiate on power output up to 5%. Any changes in performance though, are case by case sensitive on the device structure and the excitation spectrum. Specifically, it is shown that devices with thicker i-layer thickness suffering degradation, are more susceptible to performance variations caused by shifts of the illumination spectra.
Additionally, such devices show the highest over-performance, but also the lowest underperformance.

Last but not least, different methods of rating PV devices were viewed; namely the performance ratio, $PR$, and the energy yield. It was shown that the highest performance ratio of a solar cell may not necessarily correspond to the highest energy yield. Interestingly, $PR$, exhibits its maxima under relatively moderate light intensities ($200-400\text{W/m}^2$), while the maximum power output occurs under conditions of high solar intensity. Degraded devices, with relatively thick $i$-layer ($600\text{nm}$), that are prone to performance variations, will also have a tendency to show variations of the $PR$. The later is important as under specific conditions a degraded device may exhibit higher $PR$ than a non-degraded one.

Therefore, rating of all devices should be done with an understanding of the device state, but also over a long period and a wide range of illumination conditions. The performance ratio though, is an indicator of which cell performs best as compared to a strictly laboratorially controlled set of conditions. The latter is suboptimal for electricity consumers and suppliers, who buy and sell in units of energy. On the other side, the method is suitable for providing energy yield prediction, as long as long-term site specific irradiance data are used. The energy yield presents a much more robust way to rate the devices. The energy yield is directly proportional to the power output, which is the quantity, which determines the price of energy in the market. The method is impractical for the purpose of energy yield prediction, as the actual power output of the device remains unknown till measured. However, the energy yield does not depend on the device state, as the device which produces the most will also have the highest energy yield. Hence, it is suggested that PV modules should be rated on the basis of their annual energy yield, when possible.
Chapter 6 – Thesis Conclusions

In this work an opto-electrical modelling platform, which defines how light of different energy interacts with matter and specifically a-Si:H solar cells was designed. The platform was used to simulate and quantify the effects of commercial solar simulators, as well as Halogen and LED light sources on the performance of a-Si:H solar cells. A performance variation was shown to exist and to be dependant on the wavelength of the light. Such effects have not been studied and quantified before, which is a contribution to the scientific community. In addition the outdoor variation of a-Si:H solar cell performance was examined in regard to spectral changes using spectral irradiance measurements recorded over a year at Loughborough, CREST. For the first time an opto-electrical modelling platform was used to provide an energy yield simulation analysis of outdoor spectra variation on a-Si:H performance.

Although experimental methods to quantify optical-electrical losses within amorphous silicon thin-film devices have been suggested, they are difficult to implement and are subjective to experimental difficulties. On the other side modelling enables a relatively easy and inexpensive quantitative comparison of performance of alternative material properties, allows the optimisation of the physical structure of the device and its underlying loss mechanisms. Furthermore, modelling permits the direct comparison of different excitation spectra, and therefore it makes an attractive method for studying the influence of spectral effects on a-Si:H solar cell performance.

An optical model was developed, which allows the study of thin film multilayer structures with random interface roughness within a two-dimensional universe. The optical approach is ray-tracing - every beam of light is treated individually based on fundamental Physics, such as Maxwell equations. This is not the case for most models, which often initiate simplifications to avoid the analytical solution of each individual beam assuming the reflectance, or the transmittance of the front surface.

On the other hand, the suggested model is computationally demanding. Consequently, the accuracy of the examined model is subjective to its intensity calculation tolerance,
which defines the threshold level of the beams which are being rejected. Simulations have shown longer wavelengths to evade full absorption resulting in a large number of untreated beams. The main assumption of the model is that it assumes that the generation of untreated beams is qualitatively similar with the treated beams and initiates corrections to satisfy the principle of energy conservation. The magnitude of errors arising from such simplification is linked to the availability of computing memory.

An additional drawback of this model is its limitation to two-dimensions. Considering that the lateral dimensions of realistic thin-film structures are much longer and especially cell length, which in this case has been ignored, this approximation holds without loss in the generality of the solution.

The electrical collection of a-Si:H solar cells can be modelled either by equivalent circuits, or with a combination of linear components and semiconductor modelling. The first, equivalent circuit modelling, is the simplest and easiest to compute method, but it is not appropriate for modelling the behaviour of a-Si:H solar cells. The second method is based on detailed semiconductor modelling. Although it may be suitable for modelling the effects of spectral changes on a-Si:H solar cell performance, but at the same time it is impractical, as it requires a significant amount of computation and is dependent on large number of input parameters. Nevertheless, semiconductor modelling allows the inclusion of the specifics of a-Si:H solar cells such as the p-i-n junction, the dangling bond recombination and the variation of the electrostatic potential distribution within the i-layer. Crucially both factors have a significant impact on a-Si:H performance and cannot be neglected.

The conjunction of a detailed optical model and semiconductor model of the p-i-n junction enables the characterisation of the behaviour of the device under different optical excitation conditions, which may occur indoors or outdoors.

The indoor characterisation of a-Si:H solar cell devices is susceptible to the variation of the solar simulator spectrum to the standard terrestrial AM1.5G spectrum. It is shown that different light sources result in deviations in the performance evaluation of a-Si:H
solar cells. These deviations are usually small for class A solar simulators, but may be significant for Halogen or LED sources.

Firstly, it should be emphasised that the accuracy of the performance evaluation of a-Si:H solar cells is very much dependent on the solar simulator illumination spectrum. Therefore, solar simulator spectra should resemble as much as possible the standard terrestrial AM1.5G spectrum in the whole spectral region. Once a significant spectral deviation exists, the impact on the performance evaluation is not negligible.

Secondly, the magnitude of the performance deviations depends on the device state. Two factors, which have been associated with the device state have been examined in this work; the i-layer thickness of the p-i-n junction. Both have shown to have a non-negligible impact. Specifically, increasing i-layer thickness and degradation state resulted in higher performance deviations. Such deviations have been attributed to the change of the voltage dependence quantum efficiency, which affects different wavelengths differently.

In this work it was shown that the exhibited errors cannot be accurately corrected only by a simplified calibration of $J-V$ characteristics at short-circuit conditions. In these cases additional care should be taken, especially when measuring heavily degraded devices or devices with increased i-layer thickness (thicker than 400nm), as the voltage-dependent correction of the spectral mismatch should be employed. This voltage dependence of the spectral response implies that the mismatch correction should be carried out on a point by point basis.

The variations of a-Si:H solar cell performance under different outdoor spectral conditions measured at Loughborough UK during 2003-2004, has been examined. Although, similar modelling approaches have been suggested before, this is the first time a detailed opto-electrical model is used to monitor outdoor performance and its key factors, namely intensity and $APE$. This has significant importance as experimental studies so far, were affected by secondary effects such as angle of incidence, temperature and the degree of shadowing.
The key factors, which were responsible for the performance variation of a-Si:H solar cells, as compared to STC performance, are summarised as follows:

i. Light intensity is primarily responsible for a-Si:H outdoor performance. Specifically, $J_{SC}$ and power output seem to be in a linear relationship with light intensity.

ii. APE is identified as a responsible factor for the deviations observed to the linear behaviour of $J_{SC}$ to intensity. The magnitude of the outdoor spectral variation, due to APE changes is in the range of ±3% as compared to power output of the device under the AM1.5G spectrum. Its impact is more significant at high illumination intensities –when the device reaches its maximum energy yield- where increases of APE have shown an increase to $J_{SC}$ and power output.

iii. The state of the device also plays a significant role. The simulated percentage of performance variation to STC differed for a-Si:H solar cells of different i-layer thickness and level of degradation. Specifically devices with thicker i-layer, who have suffered degradation, are prone to performance variations. On the contrary thinner devices, which have not suffered degradation, show the least performance variations.

Finally, different methods of rating PV devices were viewed; namely the performance ratio, PR, and the energy yield. Interestingly, PR, exhibits its maxima under relatively moderate light intensities (200-400W/m2), while the maximum power output occurs under conditions of high solar intensity. Degraded devices, with relatively thick i-layer (600nm), that are prone to performance variations, will also have a tendency to show stronger variations of PR.

Therefore, rating of all devices should be done with an understanding of the device state. Extra care should be given in obsolete a-Si:H technologies, which tend to have thicker i-layer thickness, or devices which have suffered degradation due to prolonged light-soaking. Most importantly, performance evaluation should be carried out over a long period, which would essentially guarantee a wide range of illumination conditions and minimise the effect of seasonal over-performance or under-performance.
The performance ratio, is an indicator of which cell performs best as compared to an artificial set of operating conditions. The latter is sub-optimal for electricity consumers and suppliers, who buy and sell in units of energy. However, the method is suiting for cases where an energy prediction is necessary. On the other side, the energy yield presents a much more robust way to rate the devices. The energy yield is directly proportional to the actual power output of the device. This is the quantity, which determines the price of energy in the market. It is suggested that PV modules should be rated on the basis of their annual energy yield, when possible.

The afterword of the thesis is that spectral effects introduce performance variations in the function of amorphous silicon solar cells. The work suggests that an examination of each device in the frame of the applied spectral operation conditions should be made to safely judge its power output. So far, such statements have been empirically known to the scientific community. The scientific novelty displayed here was the use of opto-electrical modelling as a means of a rationalised comparison basis to predict and quantify power variations caused by spectral changes in a-Si:H solar cells at indoor and outdoor conditions. Furthermore, it was shown that the inclusion of the spectral sensitivity of amorphous silicon devices is essential for accurate energy yield predictions. Such calculations can be realised rapidly and inexpensively with the employment of opto-electrical modelling strategies, as long as the manufacturing characteristics of the device and the illumination spectra are known. The application of this research on future amorphous silicon power plants can potentially improve their design, as the annual energy yield, as well as the seasonal energy deficits will be predicted more accurately.
References


[50] The picture is courtesy of the Wikimedia Commons and reused under GNU free documentation license (http://en.wikipedia.org/wiki/Electromagnetic_radiation)


[105] IEC 60904-7 Photovoltaic devices. Part 7: Computation of spectral mismatch error introduced in the testing of a photovoltaic device


[115] Bandpass Filters for Oriel Solar Simulators, Solar Simulators, Light Sources, Newport Corp (2010); p.205


Bibliography


Appendix

Unless otherwise indicated all simulations use the values of the parameters listed in the following matrix.

Table XI: Parameters of the simulations used for the purpose of this thesis.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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<tbody>
<tr>
<td>Glass thickness</td>
<td>3 mm</td>
</tr>
<tr>
<td>ZnO TCO thickness</td>
<td>500 nm</td>
</tr>
<tr>
<td>μc-Si p-layer thickness</td>
<td>10 nm</td>
</tr>
<tr>
<td>a-Si:H i-layer thickness</td>
<td>250/400/600 nm</td>
</tr>
<tr>
<td>μc-Si n-layer thickness</td>
<td>10 nm</td>
</tr>
<tr>
<td>ZnO-Ag thickness</td>
<td>400 nm</td>
</tr>
<tr>
<td>ADF inerface / interface</td>
<td>cos²(θ)</td>
</tr>
<tr>
<td>ADF a-Si:H / Back Reflector</td>
<td>cos⁶(θ)</td>
</tr>
<tr>
<td>σrms interface / interface</td>
<td>10 nn</td>
</tr>
<tr>
<td>σrms n-layer / Back Reflector</td>
<td>50 nn</td>
</tr>
<tr>
<td>C</td>
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</tr>
<tr>
<td>N_C</td>
<td>10¹⁸ cm⁻³</td>
</tr>
<tr>
<td>N_V</td>
<td>10¹⁸ cm⁻³</td>
</tr>
<tr>
<td>E_g</td>
<td>1.72 eV</td>
</tr>
<tr>
<td>E_A, E_D</td>
<td>50 meV</td>
</tr>
<tr>
<td>E_mnc</td>
<td>65 meV</td>
</tr>
<tr>
<td>K</td>
<td>3·10⁻¹⁶ cm⁻³·eV⁻¹⁻⁵</td>
</tr>
<tr>
<td>g_min(0)</td>
<td>10¹⁵·10⁻⁶ cm⁻³·eV⁻¹</td>
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<tr>
<td>τ_n_B-B</td>
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</tr>
<tr>
<td>τ_n_B-B</td>
<td>3·10⁻² s</td>
</tr>
<tr>
<td>τ_n</td>
<td>10⁻⁷⁻¹⁰⁻⁹ s</td>
</tr>
<tr>
<td>τ_p</td>
<td>2·10¹⁻⁷ cm⁻¹·s⁻¹</td>
</tr>
<tr>
<td>V_th</td>
<td>5·10⁻¹⁸ cm²</td>
</tr>
<tr>
<td>σ_n</td>
<td>10⁻¹⁶ cm²</td>
</tr>
<tr>
<td>σ_p</td>
<td>100</td>
</tr>
<tr>
<td>σ_n⁺/σ_n⁻ = σ_p⁺/σ_p⁻</td>
<td>10⁻¹⁵⁻¹⁰⁻¹⁶ cm⁻³</td>
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</tr>
<tr>
<td>N_DB,as prepared</td>
<td>10</td>
</tr>
<tr>
<td>N_DB,degraded</td>
<td>10¹⁵ cm⁻³</td>
</tr>
<tr>
<td>S_n</td>
<td>7·10¹⁵ cm⁻³</td>
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<tr>
<td>S_p</td>
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<tr>
<td>R_S</td>
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