Modelling the effects of electronic parameters on the efficiency of amorphous silicon solar cells under AM1.5G spectrum

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Abstract

The purpose of this paper is to model the performance of thin film amorphous silicon (a-Si:H) solar cells under AM1.5G spectral conditions. In this work, a numerical model for the investigation of thin film amorphous silicon p-i-n cells has been developed. The light absorption is treated as a non-uniform, exponentially decaying function, which also allows to use spectral ensembles to be investigated. Based on the absorption profile, continuity and current density equations are solved numerically. This allows the calculation of the quantum efficiency of the device. The model is being validated against measurements on an a-Si:H test cell of known configuration and I-V characteristics. Then the established model is used to investigate the effects of i-layer thickness, surface recombination and electron and hole mobilities, under AM1.5G spectral irradiance, on the efficiency of a-Si thin film solar cells. The key parameters in optimising this type of a-Si:H cell are then reviewed.

1. Introduction

Solar cells are typically characterised in rather artificial conditions in the laboratory. Linking these measurements to realistic operation is the aim of this work. Realistic conditions involve having realistic chromatic light conditions, i.e. not monochromatic, and variable angles of incidences, as there is typically diffuse as well as direct irradiance incident on the photovoltaic device. Typically, there are two types of models, electrical ones, which consider effects such as doping profile and field distribution, and optical ones, which consider the effects of cell structure on optical absorption. However, in reality these two are not independent of each other.

In order to understand the behaviour of devices under realistic conditions, one needs to bring together both facets of device modelling. This paper

presents the efforts to develop a suitable electrical model. This is used for the calculation performance parameters using AM1.5G spectrum. The model is validated against experimental data and used to provide an examination of the above mentioned effects.

A simple optical model is used here, which does not allow for multiple optical path lengths, as they are achieved with light confinement provided by advanced TCOs [1]. This results in the cell thicknesses being thicker then they would be in today's devices, but these are required to achieve sufficient optical absorption for the cases simulated here. This idiosyncrasy also illustrates the importance of bringing together optical model with the electrical one.

2. Model

A typical a-Si:H solar cell consists of a p-i-n diode. The light enters the cells through the p-layer for two reasons: i) the fact that most of the incident light G_0 is absorbed close to the surface of the illuminated layer (following the Beer's law, where the intensity of the light decreases with distance exponentially in materials), and generates electron-hole pairs there, and ii) the lower mobility carriers (holes) have to be efficiently collected by the p-layer before they recombine with other electrons [2]. The charge-carrier separating electric field extends between the p- and n-layers through the i-layer. The field's intensity depends on the external voltage, the thickness of the i-layer, the illumination intensity and doping concentration. Under zero external bias conditions the direction of the field is towards the p-layer, opposite to the diffusion current for each type of charge carrier.

To derive the one dimensional distribution of free carriers, three semiconductor equations together with boundary conditions have to be used: the current density equation, continuity equation and Poisson's equation. The solution can be simplified considerably by applying the following assumptions:

i. Only the i-type layer is electrically active and collects photocarriers. The p-type and n-type layers are electrically inactive and do not contribute to carrier generation, but optically active in respect to light absorption. This is often referred to as i-layer model [3].

ii. The main recombination mechanism is considered to be dangling bond recombination [4]. In the bulk a-Si structure excessive bonds are unsatisfied and may become recombination centres for electrons and holes

iii. The third assumption is known as the "uniform-field" model. In accordance to it, the electric field through the i-layer is uniform [5].

The main approximation in this case is has negligible concentration of charges. Strictly speaking the dangling bonds in amorphous semiconductors can be in three states (D_0, D^+ and D^-). However, in the intrinsic layer of a-Si most of these bonds are in D_0 state, and therefore contribution of D^+ and D^- states to recombination may be neglected [6]. Hence Poisson's equation can be simplified, and the system can be reduced in two second order non-homogeneous ordinary differential equations..

iv. The lifetime of electrons and holes is constant through out the i-layer. This assumption is valid only when the condition $\Delta n=\Delta p \gg n_i$ is satisfied [7]. This condition may be applicable regionally in a-Si cells under illumination, but is not valid for the whole i-region, hence it is a simplification which may introduce errors.

The solving approach though becomes significantly easier and allows the investigation of a-Si solar cells, as other scientists have shown [6]. The solution of this system, its boundary conditions, and its extension to chromatic illumination are discussed in the following paragraphs.

2.1 Formulation

The simulation is based on the solution of electron and hole continuity equations (1) and (2), and electron and hole current density equations (3) and (4):

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

$$\frac{1}{q}\frac{dj_p}{dx} = G(x) - R(x) \tag{2}$$

$$j_n = q\mu_n n\xi + qD_n\frac{dn}{dx} \tag{3}$$

$$j_p = q\mu_n p\xi - qD_p\frac{dp}{dx} \tag{4}$$

where n and p are the free electron and hole densities, j_n and j_p are the electron and hole current densities, q is the elementary charge, G(x) is the generation rate as a function of position x and wavelength λ, R(x) is the recombination rate, μ_n and μ_p are the electron and hole mobilities, D_n and D_p are the electron and hole diffusion coefficients and ξ is the constant electric field. ξ is determined by equation (5).

$$\xi = \frac{V - V_{bi} + V_{fit}}{x_2 - x_1} \tag{5}$$

where V is the applied voltage, $V_{bi} = V_t \ln(N_A N_D/n_i^2)$ is the built-in potential and V_{fit} an empirical voltage determined by fitting (Table 1). The difference

V_{bi}-V_{fit} resembles the flat-band voltage which has been used by other scientists [8]. x_1 is the boundary between the p- and the i- layer and x_2 is the boundary between the i- and the n- layer. Hence, the distance x_2-x_1 represents the thickness of the i-layer.

Generation rate G is treated as a non-uniform, exponentially decaying function and is given by equation (6):

$$G(x) = G_0 a(\lambda) \exp\left[-a(\lambda) x\right] \tag{6}$$

where G_0 is the incident photon flux and $\alpha(\lambda)$ is the wavelength λ dependant absorption coefficient.

As it has been discussed above dangling bond recombination has been reported to be the main recombination mechanism in a-Si solar cells. Therefore the dangling bond controlled recombination rate R can be given by the linear form (7), given [9]:

$$R \equiv R_{DB} = \frac{n}{\tau_n} + \frac{p}{\tau_p} \tag{7}$$

where τ_n and τ_p are the capture times of free electrons and free holes respectively by neutral dangling bonds.

2.2 Boundary conditions

The system of differential equations cannot be solved without boundary conditions. The boundary conditions of the problem are defined by surface recombination as [8]:

$$J_n(x_1) = q\, s_n\left[n(x_1) - n_0(x_1)\right] \tag{8}$$

$$J_p(x_2) = q\, s_p\left[p(x_2) - p_0(x_2)\right] \tag{9}$$

$$J_n(x_2) = -q\, c_n\left[n(x_2) - n_0(x_2)\right] + J_n(x_1) \tag{10}$$

$$J_p(x_1) = -q\, c_p\left[p(x_1) - p_0(x_1)\right] + J_p(x_2) \tag{11}$$

where n_0 and p_0 are the thermal equilibrium concentrations for electrons and holes, s_n and s_p are the recombination velocities, and c_n and c_p are the collection velocities for electrons and holes respectively (Table 1).

Table 1: Flat band voltage, recombination and collection velocities used in the simulation, together with lifetimes for electrons and holes respectively.

V_{bi} - V_{fit} [V]	s_n [cm/s]	s_p [cm/s]	c_n [cm/s]	c_p [cm/s]	τ_n=τ_p [s]
0.7	$5\ 10^4$	$5\ 10^6$	10^6	10^7	10^{-6}

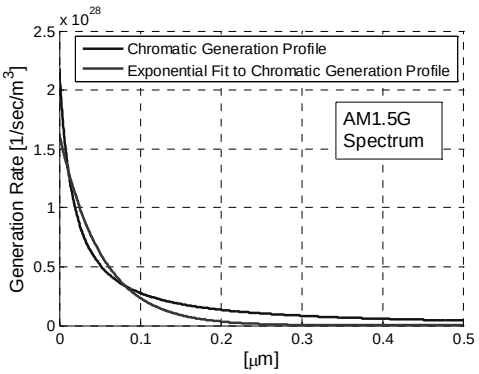

Figure 1: Chromatic generation profiles and its exponential fitting over position.

The density of majority carrier concentrations in the heavily doped regions p^+ and n^+ were taken to be in the order of 10^{20} m^{-3}. These values are significantly higher even than the photogenerated carrier profiles of the i-layer at 300K under illumination AM1.5G, where one would expect a charge carrier density in the order of 10^{13} m^{-3}.Therefore one can assume that for thermal equilibrium, the boundary majority carrier concentrations $p_{p0}(x_1)$ and $n_{n0}(x_2)$ are in the order of 10^{20} m^{-3}, and equal to N_A and N_D respecticely (Table 2).

The system of differential equations (1)-(4) can now be solved using the boundary conditions (8)-(11). The solution is processed using the "dsolve" function of the "symbolic math toolbox" of MATLAB.

2.3 Chromatic Illumination Treatment

The generation rate of monochromatic illumination can be treated analytically as a non-uniform exponentially decaying function, as described by (6). Generation rates of chromatic spectra can be expressed analytically as in (12):

$$G(x,\lambda) = \int_{\lambda_{min}}^{\lambda_{max}} G_0(\lambda)a(\lambda)\exp\left[-a(\lambda)x\right]d\lambda \qquad (12)$$

However, this expression significantly complicates the solution, and the differential system cannot be solved, hence an approximation of the generation rate is necessary. In this paper, chromatic generation profiles were treated as an exponentially decaying function, similar to (6):

$$G(x) = G_{0fit}\ a_{fit}\ \exp\left[-a_{fit}\ x\right] \qquad (13)$$

The empirical parameters G_{0fit} and a_{0fit} were determined by fitting equation (12), with the results being shown in Figure 1. The fit underestimates generation rates in the area of 10 [nm] close to the p-i and i-n boundaries, but provide a basis for understanding the effects of chromatic illumination on cell performance. This underestimation of photogeneration may result in a reduced current flow through the device, as will be shown in 3.1. It should be noted that in the current

study a-Si based cells were examined and therefore photon energies which do not exceed the a-Si bandgap energy (1.75eV) do not contribute to photogeneration.

Table 2 Structure parameters of the test cell.

Parameter	Value [Unit]
i-layer thickness	0.1 [μm]
N_D n-type	$\sim 10^{21}$ [m^{-3}]
N_A p-type	$\sim 15 \cdot 10^{21}$ [m^{-3}]

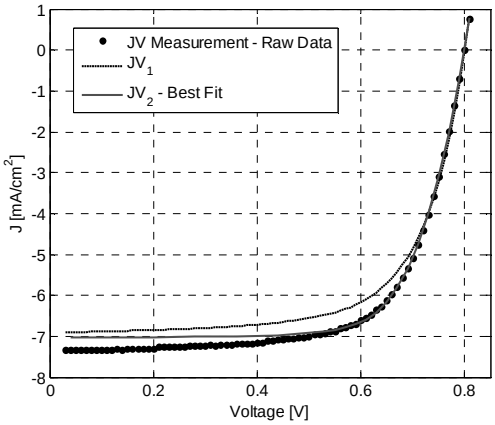

Figure 2: Comparison between an a-Si test cell and the model. Results, under STCs.

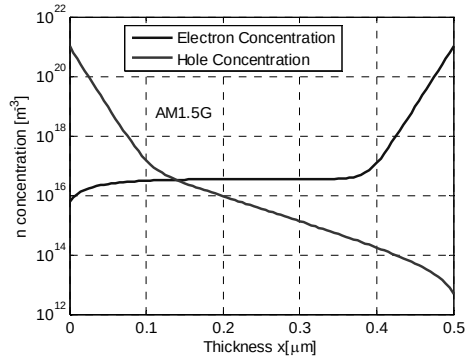

Figure 3: Free carrier distribution on a p-i-n junction, with a non-uniform excitation through the p layer, under no external bias.

3. Model validation and results

3.1 Model Validation

The model is compared to the J-V characteristics of a solar cell of known parameters. The test cell is a p-i-n a-Si cell, and its structure parameters are given in Table 2. The J-V characteristics of the cell were obtained under STCs. the simulation was realised under the same conditions. J-V_1 are the resulting simulated characteristics using the boundary conditions which have been given in Table 1. J-V_2 are the resulting characteristics fitting surface recombination and collection velocities to much best the raw data. The measure J-V characteristic are compared to the calculated results in Figure 2. A good agreement was established between J-V_2 and the raw data, as the average error does not exceed 1%. Locally near short circuit region errors may raise up to 4%. The underestimation of the short circuit current can largely be attributed to the lack of an optical model that allows for multiple passes of the light through the device.

3.2 Free carrier distribution

In this section free carrier distribution over the i-layer is calculated based on the model which was established in the previous paragraphs, and the boundary conditions given in Table 1. For the purposes of this study the spectral irradiance is considered identical to AM1.5G, and the device is considered to operate under short circuit conditions.

Figure 3 shows the free carrier distribution though the i-layer for non-uniform absorption through the p-layer. The considerable difference in the minority carrier concentrations close to the p- and n-boundaries can be explained due to the non-uniform illumination which decays exponentially as it propagates into the i-layer. This, together with the difference in mobilities between electrons and holes, is causing an asymmetric free carrier density through the i-layer. It is also noticeable that at a point closer to the p-layer, the electron and hole concentration cross each other, as e.g. also reported by [3]. The concentration of electrons and holes tends to increase steeply at 100 nm away from the p-i and i-n interfaces, respectively.

3.3 Effect of surface recombination

The values of the recombination and collection velocities are associated with the boundary conditions, therefore understanding their impact on the solution has a significant importance. To do so, multiple simulations were performed varying recombination velocities from 1 to 10^{10}. The results are shown in Figure 5, in terms of the cell quantum efficiency. The quantum efficiency (QE) is defined here as the percentage of the photons in the whole spectrum being collected as charge, which results in a low QE. However, the absolute short circuit current densities of the cells are in the order of 15-20 [mA/cm^2]. It should be also noted that in order to separate and identify the effects surface recombination velocities for electrons and holes were scaled

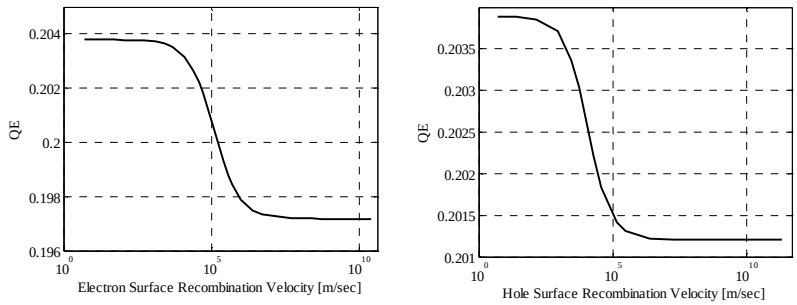

Figure 4: Comparison between the effects of surface recombination velocities of electron and holes on the quantum efficiency.

independently one at a time using the same values for collection velocities as given in Table 1.

Increasing recombination velocities lead to decreasing QE. However, in the range of recombination velocities given by [8] , the solution of the system is very stable. An increase in the recombination velocities by two orders of magnitude, leads to a significant effect on QE. Especially for recombination velocities that exceed 10^4 [cm/s] for electrons and 10^3 [cm/s] for holes QE showed a notable decrease.

Increasing collection velocities increase the calculated QE, although the effect is marginal relative to that of increased recombination velocity. The contrary variation of the collection velocities did not influence QE over 0.001 in the given range. This is the case for the 0.5μm i-layer thickness used in the simulations. Varying i–layer thickness would result in a different behaviour of collection and recombination velocities on the solution.

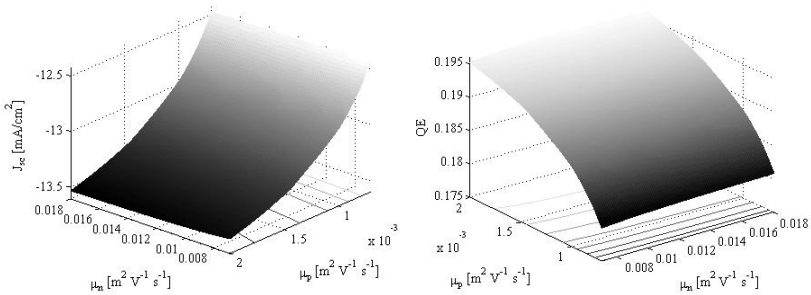

Figure 5: Comparison between the effects of electron and hole mobilities on short circuit current and quantum efficiency.

3.4 Effect of electron and hole mobilities

The material quality, and thus the electron and hole mobility, affects QE drastically. Decreasing mobilities are commonly reported to decrease current density [3], as they diminish electron and hole drift lengths. This effect is also apparent in Figure 5. It is shown that for electron and hole mobilities that exceed 0.014 [m^2 $V^{-1}s^{-1}$] and 1.8 10^{-3} [$m^2V^{-1}s^{-1}$] respectively, the cell performance is not affected significantly. However, once electron and hole mobilities surpass a critical value, a reduction of QE is seen as expected. This critical value depends strongly on the electric field strength and therefore, would vary for different i-layer thicknesses.

3.5 Effect of i-layer thickness

The role of i-layer thickness has been also examined, as illustrated in Figure 6. Expectedly, the QE will increase to a maximum value, which is achieved when virtually all the photons in the spectrally useful range are absorbed. A decrease is observed again due to majority of the charge carriers being generated close to the surface of the device. Increasing thickness will only contribute to a lesser extent. In the present simulation the optimum i-layer was close to 0.35 [μm], although this depends critically on recombination rate and lifetime-mobility product of the charge carriers. For values below 0.35 [μm] the generation is notably reduced due to the decreased total absorption, while for i-layer thicknesses that exceeded 0.35 [μm] the reducing electric field leads to decreasing quantum efficiencies. In order to suggest optimum range, each specific case has to be investigated.

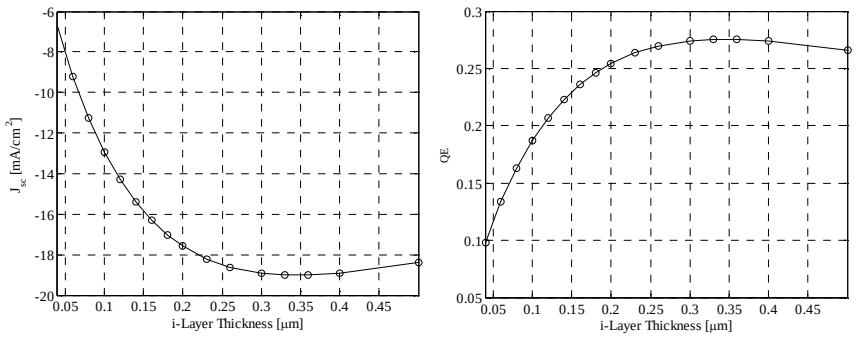

Figure 6: Effect of i-layer thickness on QE, under zero external bias conditions.

4. Conclusions

A model which can derive the free carrier distribution in a p-i-n junction, for non-uniform chromatic illumination has been developed. This model is based on continuity and current density equations, and its boundary conditions, based on surface recombination. Dangling bond recombination was considered to be the main recombination mechanism. The model was tested and good agreement was established between theoretical and experimental results under STCs. It is shown that the process of thin film a-Si cell optimisation is linked with material quality, which should be taken into account, and critical boundaries exist beyond which the performance of solar cells starts to deteriorate markedly. While here only homogenous parameters are assumed, it is clear that this is an ideal case and in reality the worst parameter will determine the performance of the cell and the cell structure should be optimised accordingly. The effect of i-layer thickness on quantum efficiency is investigated, leading to an indicative value of 0.35μm

for the given example. The p-i-n cell QE is also related to carrier mobilities, and collection and recombination velocities. It is shown that they can be chosen to be within certain safe boundaries and will not affect the device performance drastically.

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