

OPTO-ELECTRONIC MODELLING OF THIN FILM NANOCRYSTALLINE SILICON SOLAR CELLS

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Hydrogenated nanocrystalline silicon (nc-Si:H) is a mixed-phase material composed of microcrystallites and voids embedded in an amorphous matrix. This material structure makes the experimental study of the optical and electrical properties of the resulting solar cell complex. For further optimisation of the solar-cell performance a good understanding of the contribution of each layer and interface to the solar-cell performance is imperative. These contributions can be investigated by computer simulations in order to complement the limitations of experimental work. In this paper, we report the result of the investigation of optical and electrical losses in nc-Si:H solar cells using ASA numerical simulator. For this purpose, selected model parameters, which affect the solar-cell performance, are examined. In particular, the effect of p-layer activation energy is investigated in detail. Further, we examine the role of light scattering at different interfaces of nc-Si:H solar cells deposited on textured glass/ZnO:Al substrate. The scattering parameters for each interface are described in terms of the haze and the angular distribution functions for both transmitted and reflected light. The simulation results show that the activation energy of the p-layer is critical for nc-Si:H solar cell performance and mainly affect the short-circuit current density, J_{sc} . Increase in the activation energy increases the J_{sc} . With increase in the root-mean-square (rms) roughness of the TCO-p and other interfaces, the J_{sc} increases and saturates after a rms roughness value of 150 nm, according to our simulations. Using ASA, we demonstrate that low short-wavelength response of nc-Si:H solar cell can be attributed to charge carrier recombination at the p-i interface.

(Received June 21, 2012; Accepted July 9, 2012)

Keywords Hydrogenated nanocrystalline silicon, Modeling, Optical and electrical losses, Sensitivity analysis

1. Introduction

Thin film nanocrystalline silicon has become very relevant in recent times because of its use in solar cells generally and in tandem cells in particular. Its absorption ability up to the near infra red region of the solar spectrum and its band gap make it a near-perfect match for amorphous silicon solar cell in the widely applied 'micromorph' solar cell. In the tandem configuration, it serves as the bottom cell to collect the less energetic photons transmitted through the top amorphous cell and to aid tunnel-recombination at the junction between the two solar cells [1]. Being an indirect band gap material, nc-Si:H has a low absorption coefficient hence requires a relatively thick (up to 1000 nm) absorber layer and an efficient light trapping scheme for enhanced current generation within the solar cell.

Structurally, nc-Si:H is a mixed-phase material containing voids and crystals of varying sizes, shapes and orientations embedded in an amorphous matrix. Determining the exact proportion of these constituents and their contributions to the opto-electronic properties of nanocrystalline films has been a major experimental challenge. A technique such as Raman spectroscopy for example only gives information on the crystallinity make up of the material with no direct correlation to the electrical properties of the film. Implementing light trapping

approaches by the use of textured substrates, rough interfaces and reflecting back contacts enhances light absorption in the active layer of the solar cell and at the same time makes the resulting solar cell structure even more complex. This effect together with the heterogeneous nature of nc-Si:H compounds the optical and electrical behaviour of nc-Si:H solar cell, which are still not fully understood experimentally.

In the light of these research and development challenges, computer modeling has become a veritable tool for the integrated optical and electrical study of nc-Si:H solar cell. Accurate absorption and generation profiles of both amorphous and nanocrystalline solar cells have been obtained by the use of simulation models and experimental performance results (J_{sc} , V_{oc} , FF and η) have been correctly matched with simulations [2-4]. In comparison with a-Si:H whose optimization is almost saturating, much is still to be gained from the complementary experimental and computer modeling of nc-Si:H for use in tandem cells.

This paper focuses on the integrated optical and electrical modeling of p-i-n nanocrystalline silicon solar cell with the aim of investigating the sensitivity of the model parameters. These model parameters are input parameters into the simulation model, which characterize the material properties of the solar cell. The sensitivity study as presented here reveals the effects of the optical and electrical properties of each component layer of the solar cell to its overall performance and indicates areas of research focus for further improvements. The outline of this paper is as follows. In section 2, we describe the ASA simulation program given details of its characteristic features. The numerical, physical and optical models implemented in ASA are also discussed briefly. In the following section, we present a description of the experimental solar cell used for the calibration of the ASA program. For the calibration, the quantum efficiency and J-V curves of the simulated and reference solar cells are matched as a means of validating the simulation model. The last section is on the sensitivity of the model parameters. Parameters investigated include the p-layer activation energy and light scattering at the different interfaces in the solar cell. Recombination losses around the p-i interface are investigated.

2. Asa program

Advanced Semiconductor Analysis (ASA) is a one-dimensional simulation program developed by the solar cell group of the Delft University of Technology, the Netherlands. It was originally designed for the simulation of multilayered heterojunction device e.g. a-Si:H solar cell and has recently been updated for use in single junction nanocrystalline solar cell and optical systems with multi-rough interfaces. The main features of ASA include modeling of complete density of states distribution as a function of energy, which include both the extended and localized states with corresponding recombination-generation statistics [5]. The defect-pool model is used to calculate the defect-state distribution. ASA program has the main advantage of being able to run integrated optical and electrical simulation and has recently been upgraded to calculate absorption profile in the entire structure of the solar cell with scattering at rough interfaces taken into account.

A typical input statement in ASA comprises indications and specifications of the electrical and optical properties of each layer. The main features of the input statement are grid, bands, doping, model, mobility, optical, settings, etc. Continuous grading of all the input parameters as a function of position in the device can be implemented. The required output file is also specified in a print statement.

3. Model calibration

A. Optical Calibration

Calibration of a simulation model involves the fitting of the necessary input parameters (usually by iteration) so as to match the theoretical (simulated) and experimental electrical characteristics of the reference solar cell. A set of about 100 parameters describing the different optical and electrical layers of the reference solar cell are manipulated iteratively until the quantum efficiency and J-V curves of the simulated solar cell have a good agreement with the measured

ones.

For the calibration of our model, a single p-i-n junction nc-Si:H solar cell was fabricated by the rf. PECVD system used in our group. The calibration procedure was as follows: fabrication of the reference solar cell, measurements of the J-V curve and the spectral response of the solar cell under standard AM1.5 illumination and fitting the model parameters to reasonably agree with the measured characteristics [5]. The reference cell comprises p-, i-, and n- layers of thicknesses 25, 1100 and 20 nm respectively. The front TCO is 800 nm ZnO:Al and the back contact was a stack of 100 nm Ag layer upon which a 200nm Al layer was evaporated. In optical calibration, light scattering at the rough interfaces of the solar cell is taken into account.

1) Scattering parameters of the glass/ZnO:Al substrate

ZnO:Al films were deposited on Corning Eagle 2000 glass by rf magnetron sputtering. Details of the deposition method and the properties of the ZnO:Al have been published elsewhere [6]. The as-deposited film, which is 1000 nm thick, has a roughness of about 10 nm. Chemical wet etching in 0.5% diluted HCl is applied in order to introduce surface roughness. After 40 s of etching, the surface morphology is characterized by Atomic Force Microscopy from which the root-mean-square roughness of about 100 nm is obtained.

Using the total integrating sphere measurement set-up, the total and diffused transmittance and reflectance of the substrate was obtained. For the transmittance measurements, the substrate was illuminated from the glass side and on assuming that the interface between glass and the ZnO:Al layer is perfectly flat and that all incident light is transmitted, the measured parameters represent that of the ZnO:Al /air interface. In order to take the reflectance measurement, ZnO:Al surface was covered with a 50 nm Ag layer and the measurement portrays the scattering properties of the reflective air/Ag interface with the texture of ZnO:Al. From the above measurements, the haze parameters, H_t and H_r for transmitted and reflected light respectively were determined

according to the expressions: $H_t = \frac{T_{diff}}{T_{tot}}$ and $H_r = \frac{R_{diff}}{R_{tot}}$ where T_{diff} , T_{tot} , R_{diff} and R_{tot} are the

diffused and total components of the transmitted and reflected light respectively. These parameters are shown in figure 1. The haze values both for reflection and transmission is increased with the substrate roughness especially at the short wavelength region.

In order to determine the angular distribution functions, ADF_t and ADF_r of scattered light at the rough ZnO:Al/air and air/Ag interfaces respectively angular resolved scattering (ARS) measurements were carried out using red HeNe laser as light source. The intensities of the scattered light were measured at discrete angular displacements around the sample with a step of 1° varied from -90° to 90° . The ARS intensities were normalized and compared with measurements taken on a Lambertian diffuser. As seen in figure 2 the Lambertian distribution function commonly used in optical modeling over-estimates the ADF_t and ADF_r hence the need for an experimentally determined ADF values. The polar plot of ADF has a shape similar to that of a geometrical ellipse. As a result the mathematical description of ellipse has been used for the analytical approximation of the ADF [7]. The measured ADFs very much agree with the calculated.

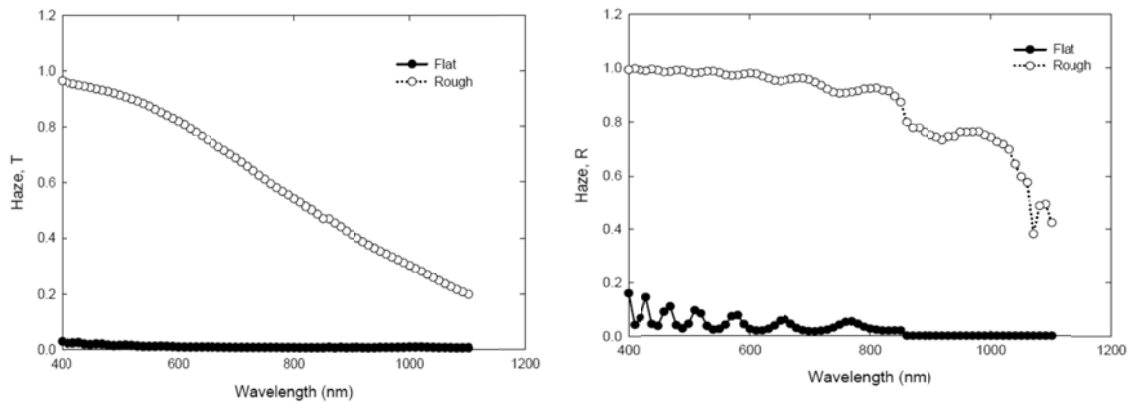


Fig. 1. Haze parameters in transmission and in reflection for flat and rough glass/ZnO:Al substrate

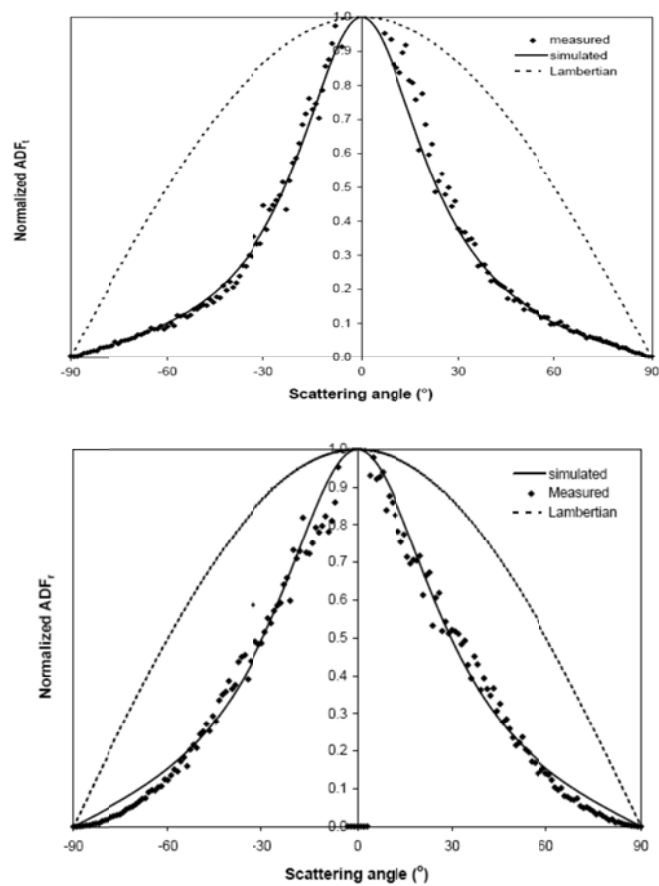


Fig. 2. The angular distribution functions ADF_t and ADF_r measured and calculated for the glass/ZnO:Al substrate.

2) Scattering parameters of the internal interfaces

The complete p-i-n structure of nc-Si:H solar cell has rough interfaces where scattering properties are difficult to be determined experimentally. On the assumption that the scattering properties of the substrate (glass/ZnO:Al) is transferred to the internal layers of the solar cell at varying degrees [7], scattering theory is applied to estimate the scattering properties of the internal interfaces.

In case of the haze parameters the scattering theory is used to obtain the H_t and H_r by correlating the rms roughness (σ_{rms}) and the refractive indices (n) of the interfacing layers in the equations [8]:

$$H_r = 1 - e^{-\left(\frac{4\pi\sigma_{rms}n_i \cos\phi}{\lambda n}\right)^2} \quad (1)$$

$$H_t = 1 - e^{-(2\pi\sigma_{rms}n_i \cos\phi_1 - n_2 \cos\phi_2)^{1.8}} \quad (2)$$

Equations (1) and (2) are further simplified by assuming that the σ_{rms} roughness is not wavelength dependent and that the angle of incidence in the incident and transmitted media is zero [4]. As a starting point, equations (1) and (2) were calibrated to validate the relevance for use in predicting the interface parameters against measured haze parameters of the ZnO:Al/air and air/Ag interfaces. The result is presented in figure 2. We assigned the same σ_{rms} roughness of 140 nm to the ZnO:Al/p and p/i interfaces while the i/n and buffer/Ag interfaces had a 50 nm σ_{rms} roughness. All other interfaces are assumed to have an ideal flat morphology.

For the ADF, the measured ADF_t and ADF_r on the substrate were approximated and analytically described by ellipse as in (3) [9]:

$$ADF_{t,r} = \frac{2kb^2}{\cos\psi_s (b^2 + \tan^2\psi_s)} \quad (3)$$

where b is the vertical radius of the ellipse believed to be dependent on the interface roughness and the scattering angle. In equation (3) k is the normalization factor. Upon the assumption that the scattering angles of the reflected light from different inclinations at rough interfaces is independent of the complex refractive indices of the interfacing layers, the ADF_r measured on the substrates is taken to be the same as the ones on the internal interfaces with similar σ_{rms} . For ADF_t , it is assumed that the angles of transmitted scattered light depend on the complex refractive indices of the interfacing layers which determine the critical angle of the total reflection affecting the light escaping cone in transmission. This effect is taken into account in calculating ADF_t by making the vertical radius of the ellipse a function of the complex refractive indices of the ZnO:Al/air interface and that of the incident and transmitted medium of the internal interlayers. The calculated ADF_t and ADF_r were transformed into a one-dimensional function in order to be incorporated in ASA by multiplying with the factor $\sin(\psi)$ for small steps in the measuring angle.

In order to validate the scattering parameters measured for the substrate and calculated for the internal interfaces, the QEs of nc-Si:H solar cells deposited on both flat and textured substrate was measured and compared with simulated QEs. The simulated QEs were obtained from the absorption in the i-layer. The measured QEs were determined from the spectral response measurement under a reverse bias voltage of -0.5 V and we assume that for this bias voltage all the photo-generated carriers are collected. Figure 3 shows the comparison of the measured and simulated QEs for both the textured and flat substrate. A good agreement is observed in the case of a rough substrate. The disagreement in the flat case could be due to recombination and absorption losses in the short wavelength region of the experimental solar cell.

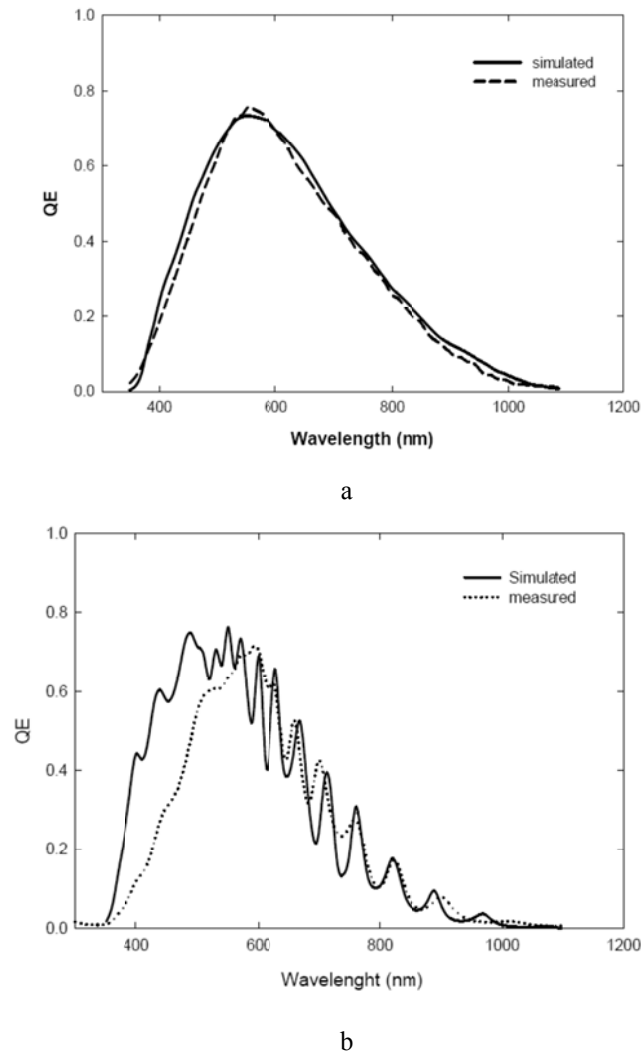


Fig. 3. Quantum efficiency curve of the nc-Si:H p-i-n solar cell deposited on glass/ZnO:Al substrate for both (a) a rough and (b) a flat substrate obtained from optical calibration

B. Electrical Calibration

For integrated optical and electrical simulation, the electrical properties of the layers that make up the solar cell are defined. Some of these input parameters, like activation energy and mobility gap, are measurable and are assigned values within experimental limits. Table 1 gives a summary of the input parameters. These parameters were maintained within known limits. The crystalline volume fraction was implemented in the model based on the effective medium approximation as proposed by Pieters et al [3].

In order to match the simulated external QE with the measured QE, the activation energy of the p- and i- layers in the input statement were adjusted. The result presented in figure 4 indicates a good matching between the measured external parameters of the solar cell and that of the simulated device.

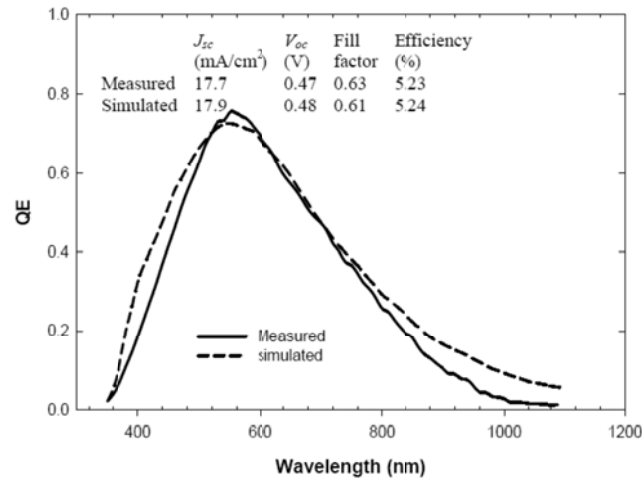


Fig. 4. External quantum efficiency obtained from electrical calibration compared with measured value taken at -0.5 V bias voltage.

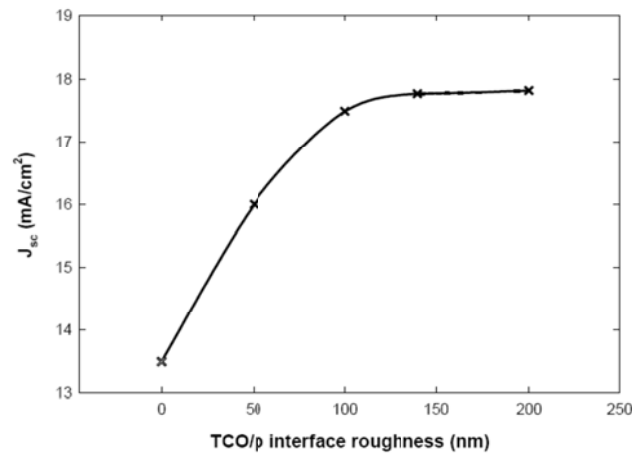


Fig. 5. Simulated TCO/p interface roughness contribution to J_{sc} of nc-Si:H solar cells.

4. Sensitivity studies

B. TCO-p and p-i interface roughness

In Figure 5, the simulated effect of the TCO/p interface roughness on J_{sc} is presented. In this simulation the p-i interface is assumed to have the same rms roughness as the TCO/p interface. We see that the J_{sc} increases with increasing TCO/p roughness and saturates around rms value of 150 nm. The percentage increase in J_{sc} drops in going from a lower σ_{rms} to a higher value.

Table 1 Set of input parameters used for the electrical calibration of nc-Si:H solar cell.
Abbreviations: DOS, density of states; CB, conduction band; VB, valence band; SD, standard deviation; DB, dangling bond

Parameter	<i>p</i> -layer	<i>i</i> -layer	<i>n</i> -layer
Thickness (nm)	24	1100	20
Mobility gap (eV)	1.18	1.18	1.75
Electron affinity (eV)	4.05	4.05	3.90
Effective DOS in CB (m^{-3})	1.25×10^2 ₅	1.25×10^2 ₅	4.0 $\times 10^{26}$
Effective DOS in VB (m^{-3})	0.62×10^2 ₅	0.62×10^2 ₅	4.0 $\times 10^{26}$
Dielectric constant	11.9	11.9	11.9
Activation energy (eV)	0.10	-	0.10
Electron mobility ($\text{m}^2\text{V}^{-1}\text{s}^{-1}$)	5×10^{-3}	5×10^{-3}	2×10^{-3}
Hole mobility ($\text{m}^2\text{V}^{-1}\text{s}^{-1}$)	1.5×10^{-3}	1.5×10^{-3}	0.5×10^{-3}
DOS at CB mob. Edge ($\text{m}^{-3}\text{eV}^{-1}$)	2.8×10^{26}	2.8×10^{26}	7.0 $\times 10^{27}$
DOS at VB mob. Edge ($\text{m}^{-3}\text{eV}^{-1}$)	1×10^{26}	1×10^{26}	5×10^{27}
CB tail characteristic energy (eV)	0.031	0.031	0.07
VB tail characteristic energy (eV)	0.031	0.031	0.08
Electron capture rate in neutral tail states ($\text{m}^{-3}\text{eV}^{-1}$)	5×10^{-15}	5×10^{-15}	0.7×10^{-15}
Hole capture rate in neutral tail states ($\text{m}^{-3}\text{eV}^{-1}$)	5×10^{-15}	5×10^{-15}	0.7×10^{-15}
Electron capture rate in positively charged tail states ($\text{m}^{-3}\text{eV}^{-1}$)	50×10^{-15}	50×10^{-15}	7×10^{-15}
Hole capture rate in negatively charged tail states ($\text{m}^{-3}\text{eV}^{-1}$)	50×10^{-15}	50×10^{-15}	7×10^{-15}
Length of the VB tail (eV)	0.9	0.9	0.9
Length of the CB tail (eV)	0.9	0.9	0.9
SD of the Gaussian DB distribution	0.15	0.15	0.15
Defect concentration (m^{-3})	3×10^{22}	2×10^{22}	2×10^{22}
Levels in which DB is discretised	40	40	40

C. Effect of *p*-layer activation energy

In Figure 6 the blue response is further investigated by simulation and is shown to depend slightly on the activation energy of the *p*-layer. The activation energy here represents the energy difference between the Fermi level and the valence band edge. The blue response decreases with decreasing activation energy of the *p*-layer, leading to a drop of the short-circuit current density. We associate this to increased charge-carrier density and attendant recombination around this interface. As shown in Figure 7, the recombination rate increases as the *p*-layer activation energy decreases. The other parameters of the solar cell also decrease slightly with decreasing activation energy and increasing charge-carrier recombination.

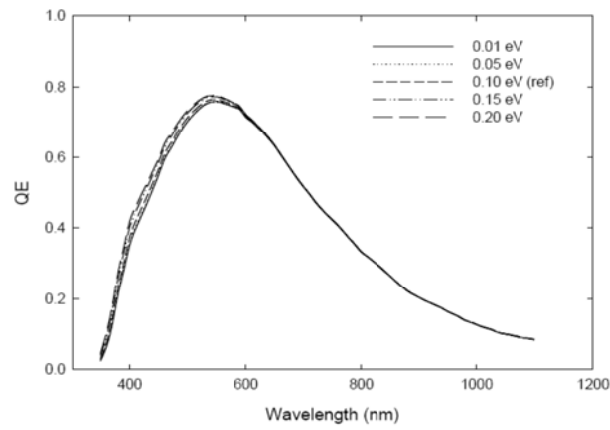


Fig. 6. External quantum efficiency of nc-Si:H solar cells as a affected by the p-layer activation energy

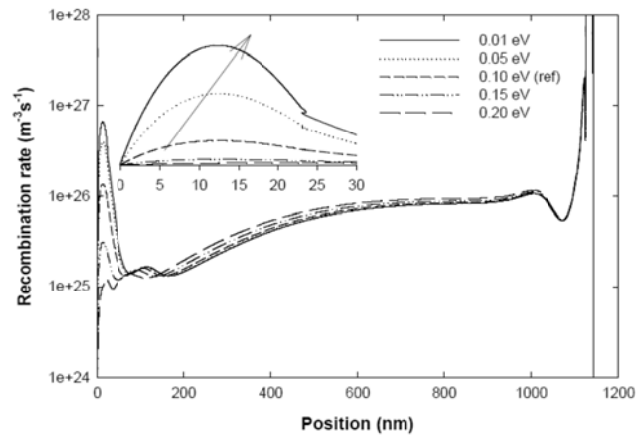


Fig. 7. Recombination rate profile of the solar cell for varying p-layer activation energy.

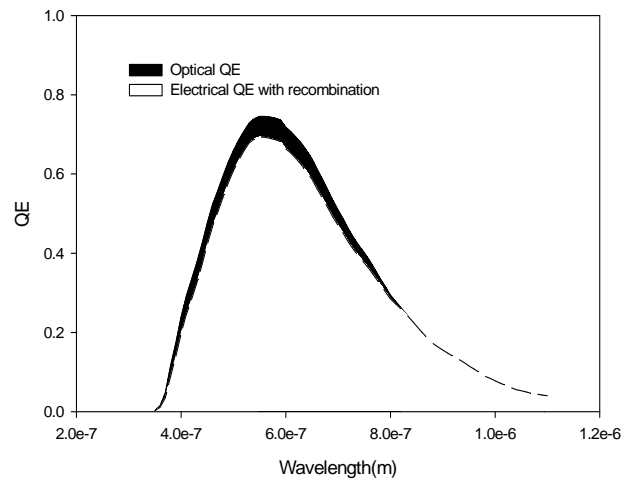


Fig. 8. A comparison between optical quantum efficiency and electrical QE indicating losses (shaded area) due to recombination in the nc-Si:H solar cell.

D. Charge carrier recombination within the layers and at the interfaces

Ideally, in a solar cell all photo-generated carriers are collected. If that is the case, the electrical quantum efficiency is equal to the optical quantum efficiency.

However, in reality due to carrier transport from the point of generation to the external contacts, recombination occurs either within the bulk or at the interfaces of the layers of the solar cell. We demonstrate this effect in figure 8. In this figure, the regions where the optical quantum efficiency is greater than the electrical quantum efficiency indicate electrical losses due to recombination.

Conclusion

We have successfully calibrated our ASA program for modeling nc-Si:H solar cell. Light scattering at the interfaces of the solar cell was implemented in terms of the angular distribution function and the haze parameters. Increasing the TCO-p interface roughness leads to increase in J_{sc} up till saturation at around a rms roughness value of 200 nm.

The p-layer activation energy affects the short circuit current density of the solar cell. At high activation energy less recombination takes place and a higher current and open circuit voltage is obtained which increases the overall efficiency of the solar cell. We have demonstrated using integrated optical and electrical simulation that the difference between optical and electrical quantum efficiency can be linked to carrier losses in recombination within the layers and interfaces of the solar cell.

References

- [1] A. V. Shah, J. Meier, E. Vallat-Sauvain, N. Wyrsh, U. Kroll, C. Droz and U. Graf, *Solar Energy Materials and Solar Cells* **78**, 468 (2003).
- [2] A. Campa, J. Krc and M. Topic, *J. App. Phys.* **105**, 083107 (2009).
- [3] B. E. Pieters, H. Stiebig, M. Zeman, R. A. C. M. M. van Swaaij, *J. App. Phys.* **105**, 044502 (2009).
- [4] J. Krč, M. Zeman, F. Smole and M. Topic, *Thin solid films* **451-452**, 298-302 (2004).
- [5] M. Zeman, J. A. Wilemen, S. Solntsev and J. W. Metselaar, *Solar Energy Materials and Solar Cells* **34**, 557 (1994).
- [6] A.M.K. Dagamseh, B. Vet, F.D. Tichelar, P. Sutta and M. Zeman, *Thin solid films* **516**, 7844-7850.
- [7] J. Krc, M. Zeman, O. Kluth, F. Smole and M. Topic, *Thin solid films* **426**, 296-304 (2003).
- [8] M. Zeman, R. A. C. M. M. van Swaaij, J. W. Metselaar, *J. Appl. Phys.* **88**, 6436 (2000).
- [9] J. Krč, M. Zeman, F. Smole and M. Topic, *J. Appl. Phys.* **92**(2), 749 (2002).