

MODELING AND SIMULATION OF OPTICAL CHARACTERISTICS IN A TEXTURED A-SI THIN FILM SOLAR CELL USING THE TRANSFER MATRIX METHOD

Florin DRAGAN¹, Andrei BADEA¹, Laurentiu FARA^{1,2}

Abstract. *A simulation of a thin film hydrogenated amorphous silicon cell was developed, in order to demonstrate the use of the transfer matrix method, TMM, with diffusive interfaces to model a textured a-Si solar cell. A quantum efficiency comparison between experiment and simulation of thin film a-Si:H solar cell was performed. We have implemented a self-consistent optoelectronic model for simulation of solar cells with rough textured interfaces.*

Key words: thin film solar cells, transfer matrix, quantum efficiency

1. Introduction

Worldwide growth of photovoltaics has been fitting an exponential curve for more than two decades [1-3]. During this period of time, photovoltaics (PV), also known as solar PV, has evolved from a pure niche market of small scale applications towards becoming a mainstream electricity source [4]. There that is being made a rapid progress with inorganic thin-film photovoltaic (PV) technologies, both in the laboratory and in industry. While amorphous silicon based PV modules have been around for almost 30 years, recent industrial developments include the first polycrystalline silicon thin-film solar cells on glass and the first tandem solar cells based on stacks of amorphous and microcrystalline silicon films [5-7]. Optical modeling has become a powerful tool for analyzing the optical properties of the thin-film solar cells. To model the complex optical behavior in the multi-layer optical systems with rough interfaces, such as a-Si solar cells, accurately, there should be taken into account both the interference effects and light scattering [8]. To optimize the performance of the solar cells by taking advantage of the enhanced light absorption, one needs to understand the influence of light scattering on the absorption profile in the solar cell. We would expect that the light is completely scattered, or in other words, diffused in the solar cell after passing through several rough interfaces. However, in wavelength-dependent spectral response and total reflection measurements on the solar cells, a moderately pronounced interference pattern can be observed. This indicates that besides the scattered light, which propagates incoherently in different directions, there is still a significant amount of specular light in the structure that propagates coherently.

¹University Polytechnic of Bucharest, Physics Department, Academic Centre for Optical Engineering and Photonics, Bucharest, Romania.

²Academy of Romanian Scientists, Bucharest, Romania.

To model the light scattering process in the solar cells accurately, the optical model needs to be calibrated well, i.e., the input scattering parameters of the model have to reproduce the available experimental data as precise as possible [9].

2. Materials and method

2.1. Materials

Amorphous silicon (a-Si) has been used as a photovoltaic solar cell material for devices which require very little power, such as pocket calculators, because their lower performance compared to conventional crystalline silicon (c-Si) solar cells is more than offset by their simplified and lower cost of deposition onto a substrate. The first solar powered calculators were already available in the late 1970^s [10].

More recently, improvements in a-Si construction techniques have made them more attractive for large-area solar cell use as well. Here their lower inherent efficiency is made up, at least partially, by their thinness – higher efficiencies can be reached by stacking several thin-film cells on top of each other, each one tuned to work well at a specific frequency of light. This approach is not applicable to c-Si cells, which are thick as a result of their construction technique and are therefore largely opaque, blocking light from reaching other layers in a stack.

The main advantage of a-Si in large scale production is not efficiency, but cost. Amorphous silicon cells use only a fraction of the silicon needed for typical c-Si cells, and the cost of the silicon has historically been a significant contributor to cell cost. However, the higher costs of manufacture due to the multi-layer construction have, to date, made a-Si unattractive except in roles where their thinness or flexibility are an advantage.

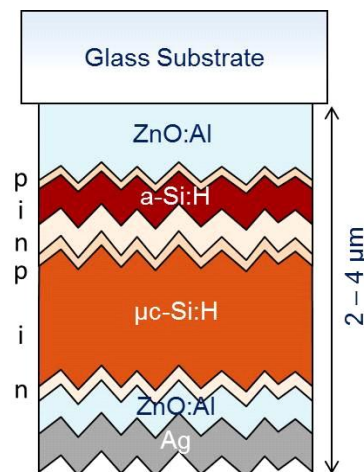


Fig. 1. Schematic of a state-of-art p-i-n a-Si:H solar cell on a glass superstrate [12].

Typically, amorphous silicon thin-film cells use a p-i-n structure. Typical panel structure includes front side glass, TCO, thin-film silicon, back contact, polyvinyl butyral (PVB) and back side glass. Uni-Solar, a division of Energy Conversion Devices produced a version of flexible backings, used in roll-on roofing products.

The structure of a state-of-art p-i-n a-Si:H solar cell on a soda-lime glass superstrate is shown in Figure 1. The front TCO (ZnO:Al) must have a low sheet resistance of about $10 \Omega/\text{sq}$ and a high optical transmission for visible wavelengths [11,12].

2.2. Method

Texturing is often used to improve light trapping in thin film solar cells. [13,19]. The textured surfaces act to scatter the light in oblique angles lengthening the optical path and effectively trapping a greater percentage of light within the thin layers [14,15].

Numerical simulation including self-consistent inclusion of optical and electrical simulation has been an important tool in optimization of solar cell designs. However texturing is problematic for numerical optoelectronic simulation of thin film solar cells. Purely geometric simulation such as Ray Tracing Method (RTM) is not suitable since it ignores interference effects occurring in devices with material layers with thicknesses on the order of the wavelength of the incident light. Also it is difficult to properly describe randomly textured surfaces geometrically [16, 17]. On the other, hand coherent modeling using Transfer Matrix Method (TMM) ignores the effects of surface texturing. Finite difference time methods could also be used but at an enormous sacrifice in computation time and with problems with periodicity and non-normal incidence.

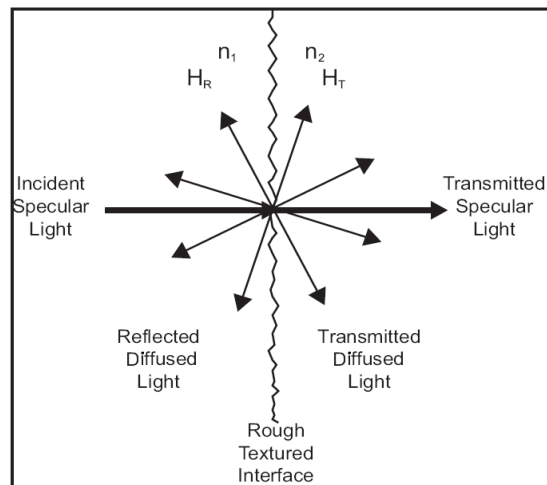


Fig. 2. Relationship between the haze functions and the specular and diffused light at a textured interface.

An approach that accounts for both the coherent propagation of specular light as well as the diffuse propagation of incoherent light occurring at the rough interfaces in the device has been proposed [8, 18]. In this approach, coherent light is modeled using the transfer matrix method while incoherent light is modeled using geometric methods. This model is incorporated into the Luminous simulator in the Silvaco ATLAS framework [7] for self-consistent optical propagation and drift-diffusion simulation of photo-detection problems.

The relation between coherent and incoherent light is defined by a set of haze functions defined at each textured interface. The haze functions H_T and H_R as illustrated in Figure 2, define the ratio of transmitted diffuse intensity to the specular incident intensity and the ratio of the reflected diffuse intensity to the specular incident intensity.

The haze functions are calculated by the expressions:

$$H_T = 1 - \exp \left[- \left(\frac{4\pi\sigma \cdot CT \cdot |n_1 - n_2|}{\lambda} \right)^{NT} \right] \quad (1)$$

$$H_R = 1 - \exp \left[- \left(\frac{4\pi\sigma \cdot CT \cdot n_1}{\lambda} \right)^{NR} \right] \quad (2)$$

Table 1. Default parameter values for the haze functions

<i>No.</i>	<i>Parameter</i>	<i>Value</i>	<i>Units</i>
1	CR	1	
2	CT	0.5	
3	NR	2	
4	NT	3	
5	σ	20	nm

where λ is the optical wavelength, CT, CR, NT, NR and σ are user definable model parameters. The parameter σ is a measure of the mean feature size at the interface. The default values of the model parameters are given in Table 1.

Figure 3 shows example calculations of the haze functions versus wavelength for various values of σ .

The diffuse light is reflected and transmitted in random directions from the interface. The distribution of diffuse light can be described by an angular distribution function, ADF. The ATLAS-Luminous simulator supports several user selectable ADFs as summarized in Table 2.

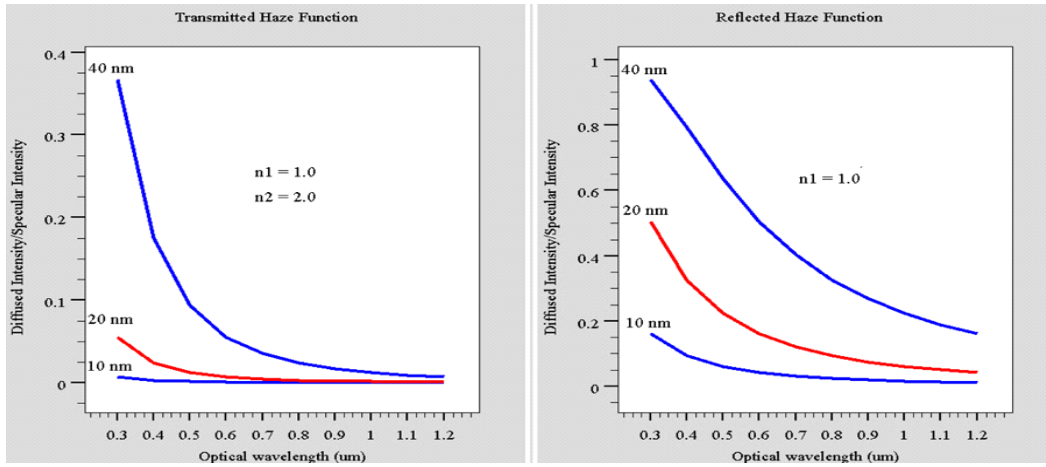


Fig. 3. Example haze functions as a function of wavelength for various σ [7].

Table 2. Un-normalized Angular Distribution Functions in Luminous.

No.		$ADF(\Phi)$
1	Constant	1
2	Triangle	$1 - \frac{2\Phi}{\pi}$
3	Gauss	$\exp\left(\frac{-\Phi^2}{2-DISPERSION}\right)$
4	Lorenz	$\exp\left(\frac{1}{\Phi^2 + DISPERSION^2}\right)$
5	Lambert	$\cos(\Phi)$
6	Ellipse	$\frac{\cos(\Phi)}{\cos^2(\Phi) + \left(\frac{0.5}{SEMIMINOR}\right)^2 \sin^2(\Phi)}$

In Table 2, Φ is the angle of propagation with respect to the normal to the interface and the ADFs are un-normalized. Normalization insures conservation of intensity derived from the haze functions above.

The geometrical contribution of the diffuse light is accounted for in the calculated photogeneration rate given in equation 3 where P_0 is the intensity at the interface, y is the distance normal to the interface and α is the absorption coefficient.

$$G(y) = 2 \int_0^{\frac{\pi}{2}} P_0 ADF(\Phi) \alpha e^{-\frac{\alpha y}{\cos \Phi}} d\Phi \quad (3)$$

Reflection and refraction of diffuse light at subsequent interfaces is modeled using the Fresnel equations.

3. The simulation software – Silvaco ATLAS

Atlas is a 2D and 3D device simulator that performs DC, AC, and transient analysis for silicon, binary, ternary, and quaternary material-based devices. Atlas enables the characterization and optimization of semiconductor devices for a wide range of technologies.

Luminous 2D/3D is an advanced device simulator specially designed to model light absorption and photogeneration in planar and non-planar semiconductor devices. Solutions for general optical sources are obtained using geometric ray tracing or beam propagation methods. These features enable Luminous 2D/3D to account for arbitrary topologies, internal and external reflections and refractions, polarization dependencies, dispersion and coherence effects. Luminous 2D/3D is fully integrated within Atlas with a seamless link to other Atlas device technology modules [19,24].

Solar cell characteristics, such as collection efficiency, spectral response, open circuit voltage and short circuit current can be extracted with Luminous 2D/3D.

4. Results and discussions

A thin film hydrogenated amorphous silicon cell was simulated using the Silvaco ATLAS simulation software. The device consists of a one half micron thick textured transparent conducting oxide, on top of p/i/n textured layers of amorphous silicon of thicknesses 9nm/650nm/20nm all on top of 300 nm of silver, shown in Figure 4.

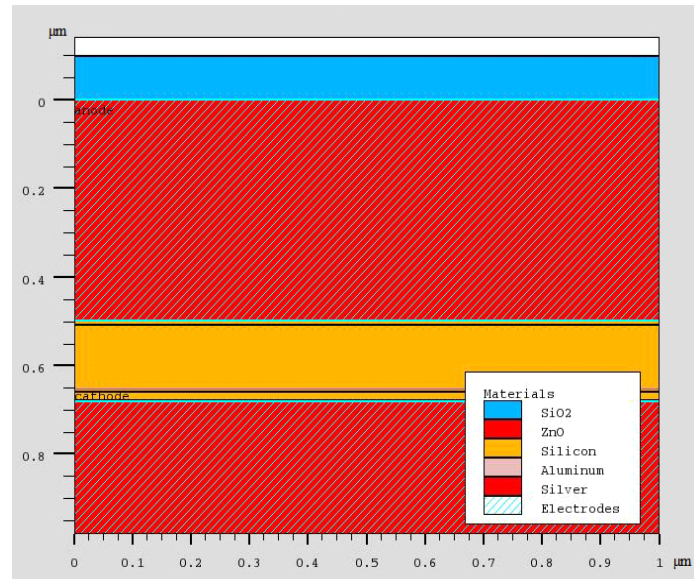


Fig. 4. The structure of a thin film a-Si:H solar cell

In the following, the steps of the simulation in ATLAS, together with the obtained results, are presented.

First we specify a mesh of 0.1 square meter. Since the structure is essentially one dimensional we ignore variations if x and z.

Next, we introduce a set of material layers comprising the solar cell device. It is important to introduce all material layers even if they have little or no electrical effect since they will have significant effects on the transfer matrix analysis used to model the optical problem.

Next, we define several of the interfaces as diffusive with certain haze function parameter specifications and angular distribution functions.

Also, we define the complex index of refraction for some of the active layers using tabular data.

For the metals and oxide we use the Sopra data base for the default complex index of refraction [20, 21].

We plot the complex index of refraction data (see Figure 5).

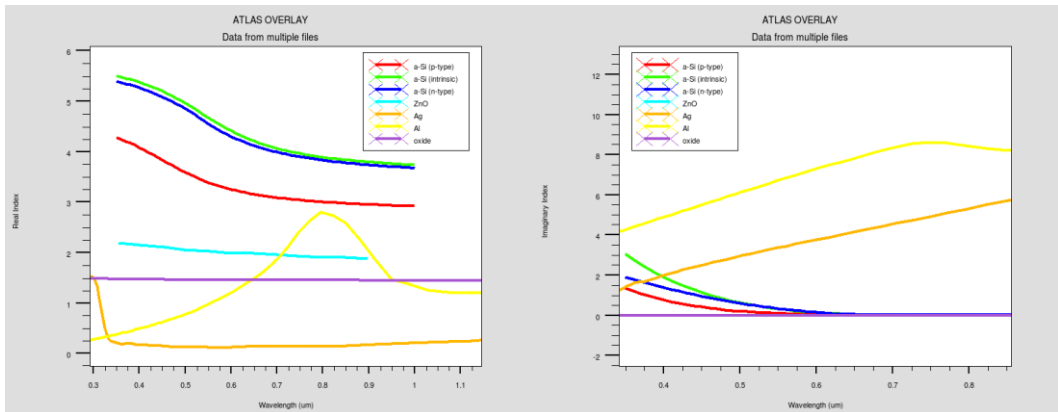


Fig. 5. The plotted complex index of refraction data:
a) real; **b)** imaginary.

We model the optical source as coming from above the device normal to the top surface. We define the source as monochromatic with an arbitrary wavelength since we will be performing spectral analysis later. We also enable the transfer matrix with diffuse interfaces.

We save the spectral response for the device to a log file. We can extract useful performance measures using the EXTRACT statements.

Finally, we can plot the results as compared against measurement. Figure 6 shows excellent comparison between experiment and simulation for this device [22-24].

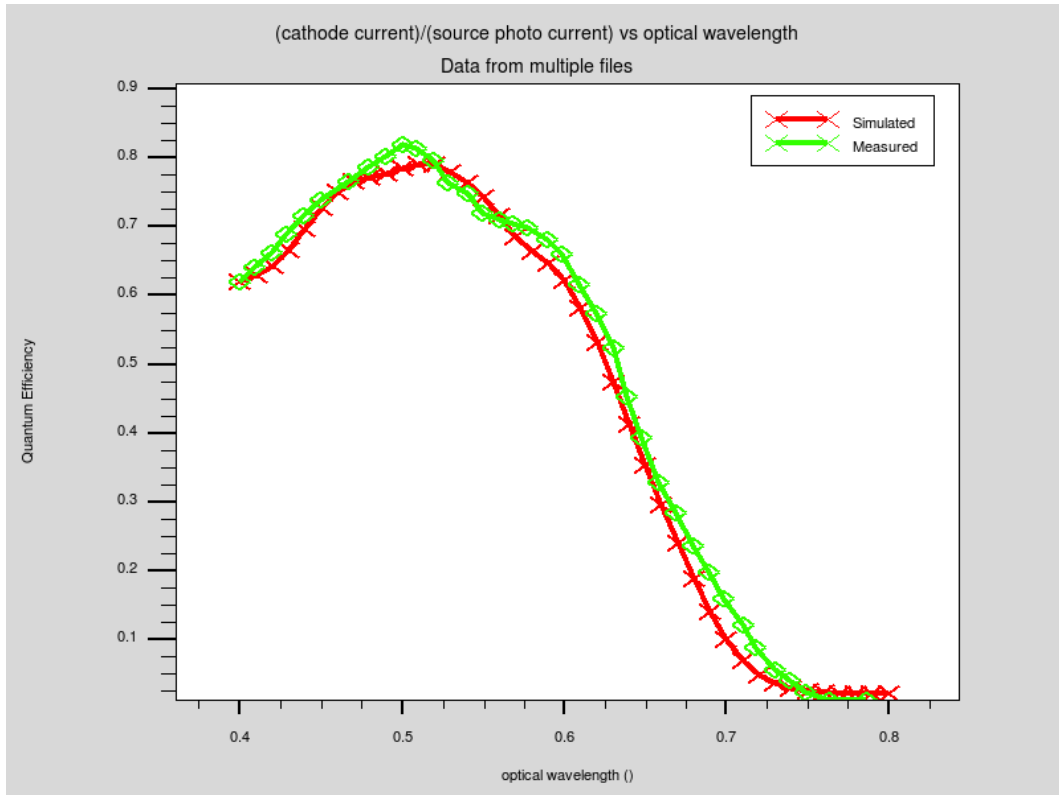


Fig. 6. Quantum Efficiency comparison between experiment and simulation of a thin film a-Si:H solar cell.

5. Conclusions

This simulation demonstrates the use of the transfer matrix method, with diffusive interfaces to model a textured a-Si solar cell. This approach is equally applicable to other types of textured thin film cells such as CIGS cells. The keys to this simulation are the use of the transfer matrix method to account for the coherent interference in the thin films and the use of diffusive interfaces to account for the effects of light trapping in the textured surfaces.

This example also shows the importance and methodology of including conducting layers in the simulation using the transfer matrix method. We have implemented a self-consistent optoelectronic model for simulation of solar cells with rough textured interfaces.

This simulator combines simulation of specular and diffuse light with haze functions describing the relation between the light intensities and angular distribution functions describing the diffuse dispersion of light.

The comparison with experiment gives good accuracy.

REFERENCES

- [1] Fara, L., Yamaguchi, M., *Advanced Solar Cell Materials, Technology, Modelling, and Simulation*. IGI Global Publishing House, USA., **2013**.
- [2] Fara, L., Diaconu, A., Dragan, F., *Trends, Challenges and Opportunities in Advanced Solar Cells Technologies and PV Market*, Journal of Green Engineering 5, 157-186, **2016**.
- [3] Diaconu, A. et al., *Results in Sizing and Simulation of PV Applications Based on Different Solar Cell Technologies*, Journal of Power and Energy Engineering 5(1), 63, **2017**.
- [4] Poortmans, J., Arkhipov, V., *Thin Film Solar Cells: Fabrication, Characterization and Applications*, John Wiley & Sons, 502 pp, **2006**.
- [5] Sterian, P., *Photonics* (in Romanian), 580 pp., Printech, **2000**.
- [6] Popescu I.M. et al., *Applications of Lasers* (in Romanian), 521 pp., Technical Publishing House, **1979**.
- [7] ATLAS User's Manual – Device Simulation Software, SILVACO, Santa Clara, USA, **2016**.
- [8] Aberle, A. G., *Thin Film Solar Cells*, Thin Solid Films 517, pp. 4706–4710, **2009**.
- [9] Krc, J. Zeman M., Smole, V., Topic, M., *Optical Modeling of a-Si:H Solar cells deposited on textured glass/SnO₂ substrates*, J. Appl. Phys., Vol. 92, No. 2, pp. 749-755, July **2002**.
- [10] Wesoff, E., *The End of Oerlikon's Amorphous Silicon Solar Saga*, Greentech Media, January 31, **2014**.
- [11] Song, D., Widenborg, P., Chin, W., Aberle, A. G., Sol. Energy Mater. Sol. Cells, vol. 73, pp. 1-20, **2002**.
- [12] ****Compound semiconductors and silicon solar cells for industrial applications*, https://www.helmholtz-berlin.de/forschung/programm/ee/next-pv/e-ip-nextpv111_en.html. Accessed May **2017**
- [13] Muller, J, Rech, B., Springer, J., Vanecek, M., *TCO and light trapping in silicon thin film solar cells*, Solar Energy, Vol. 77, Issue 6, pp 917–930, **2004**.
- [14] Kluth, O., Rech, B., Houben, L., Wieder, S., Schope, G., Beneking, C., Wagner, H., Loffi, A., Schock, H. W., *Texture etched ZnO:Al coated glass substrates for silicon based thin film solar cells*, Thin Solid Films, Vol. 351, Issues 1–2, pp. 247–253, **1999**.
- [15] *Textured Thin-film Solar Cell Simulation*, Simulation Standard, Vol. 19, No. 3, pp 11-13, September **2009**.
- [16] Becker, C., Preidel, V., Amkreutz, D., Haschke, J., Rech, B., *Double-side textured liquid phase crystallized silicon thin-film solar cells on imprinted glass*, Solar Energy Materials and Solar Cells, Vol. 135, pp 2–7, **2015**.
- [17] Tan, H., Moulin, E., Si, F. T., Schüttauf, J. W., Stuckelberger, M., Isabella, O., Haug, F. J., Ballif, C., Zeman, M., Smets, A. H. M., *Highly transparent modulated surface textured front electrodes for high-efficiency multijunction thin-film silicon solar cells*, Prog. Photovolt. Res. Appl., Vol. 23, pp. 949–963, **2015**.

- [18] Zeman, M., van Swaaij, R., Metzelaar, J., *Optical modeling of a-Si:H solar cells with rough interfaces: Effect of back contact and interface roughness*, J. Appl. Phys., Vol. 88, No. 11, pp. 6436-6443, 1 Dec. **2000**.
- [19] Eliade Stefanescu et al, *Study on the fermion systems coupled by electric dipol interaction with the free electromagnetic field*, Proc. SPIE 5850, Advanced Laser Technologies 2004, p. 160, August 05, **2005**.
- [20] Fara, L., et al. *Building Integrated Photovoltaic (BIPV) systems in Romania. Monitoring, modelling and experimental validation*, JOURNAL OF OPTOELECTRONICS AND ADVANCED MATERIALS 15.1-2 (**2013**): 125-130.
- [21] Fara, Silvian et al., *New Results in Optical Modelling of Quantum Well Solar Cells*, International Journal of Photoenergy, **2012**.
- [22] Sterian, Paul E. *Transmisia optică a informației*. Editura Tehnică, **1981**.
- [23] Manaila-Maximean, D., C. Red, Manaila-Maximean D., S. Klosowicz, KL Czuprynski, JM Gill, and M. Alexander. *Polymer-Dispersed cholesteric liquid crystals reflecting in the infrared region* Molecular Crystals and Liquid Crystals 417, no. 1, pp. 199-205, (**2004**).
- [24] ***sspectra.com/sopra.html. Accessed May **2017**.