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Optical Modeling of Ultrathin Silicon Solar Cells with PC1D

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We show that the optical diffusion model embedded in the numerical simulation program PC1D systematically underestimates light-generated currents in thin textured Si solar cells. The demonstration exploits the exact analytical solution to minority-carrier transport in uniformly doped regions and the fact that, at the first pass of internal light, the average optical propagation angle, θ, with respect to the device normal is determined by surface texture. We provide a simple correction procedure to remove the aforementioned systematical error. One can so reliably model with PC1D the optical performance of textured thin devices at standard Lambertian regimen ($\theta = 60^\circ$ at all wavelengths, λ) that starts at either the first or the second pass of trapped light. We exploit such a possibility to scrutinize with PC1D a reported non-standard Lambertian optical model, where θ varies with λ.

1. Introduction

There is increasing interest in designing ultrathin Si solar cells with active layer thickness of a few micrometers because of their reduced cost of production compared to conventional devices. In such thin films, efficient light absorption is achieved with both broadband antireflection coatings and effective light-trapping structures.[1] In the present work, we deal with light trapping.

Light trapping depends on both internal reflectance and average propagation angle, θ, with respect to the device normal of the light crossing the device. The limit for θ occurs at standard Lambertian optics, where $\theta = 60^\circ$ at all wavelengths, λ. The value of θ may vary at each pass of light across the considered device. Depending on the capability of the front and rear surfaces of diffusing light rays, $\theta = 60^\circ$ can be reached at the first, second, or third pass of light across the device. In the present work, we show that the first two cases can be modeled in ultrathin Si solar cells by the numerical simulation program PC1D,[2] provided that an optical diffusion model embedded in the program is taken into account. This diffusion model is activated when one or both internal surfaces are imposed to be optically diffusive.[3]

We show that the PC1D diffusion model underestimates light-generated currents at low device thickness. A simple correction procedure is though provided, which allows simulating the performance of textured Si solar cells with PC1D safely at any device thickness. PC1D can so become a very useful tool in designing ultrathin Si solar cells. In the present work, however, the new capabilities of PC1D that come with the aforementioned correction procedure are exploited for theoretical purposes. A reported non-standard Lambertian optical model,[4] where θ varies with λ, is shown to be in fact practically equivalent to a model, where standard Lambertian optics ($\theta = 60^\circ$ at any λ-value) is reached at the second optical pass, while, at the first pass, θ is determined by the facet angle of common surface texture.

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2. Standard Lambertian Optics in PC1D

In the standard approach to Lambertian optics, θ is assigned at any λ-value the average value, $\theta_m = 60^\circ$, calculated with[4]

$$e^{-\alpha W/\cos\theta_m} = 2\int_0^{\pi/2} \sin\theta\cos\theta e^{-\alpha W/\cos\theta} d\theta$$

where α is the absorption coefficient and W the device thickness, at $\alpha W << 1$.

In the following, θ will be denoted as θ_1 at the first optical pass and θ_n at the second and successive optical passes (see **Figure 1**). $\theta = 60^\circ$ at all optical passes across a Si sheet can be consequently achieved by simultaneously assigning $\theta_1 = 60^\circ$ and $\theta_n = 60^\circ$. PC1D allows assigning θ_1 through opportune adjustment of the facet angle, δ (see Figure 1). At PC1D default value for refractive index, we have $\theta_1 = 60^\circ$ at $\delta = 75.705^\circ$. At $\theta_1 = 60^\circ$, $\theta_n = 60^\circ$ is simultaneously assigned in PC1D by simply checking "specular" in both the rear- and front-surface sections of the "Reflectance" dialog box.

In PC1D, on the other hand, $\theta_n = 60^\circ$ can be also imposed by checking "diffuse" in the aforementioned rear-surface section of the "Reflectance" dialog box.[3] In this case, $\theta_n = 60^\circ$ is set regardless of θ_1.

In PC1D, however, checking "diffuse" in the rear-surface section of the "Reflectance" dialog box triggers automatically a built-in optical model called "diffusion model".[3]

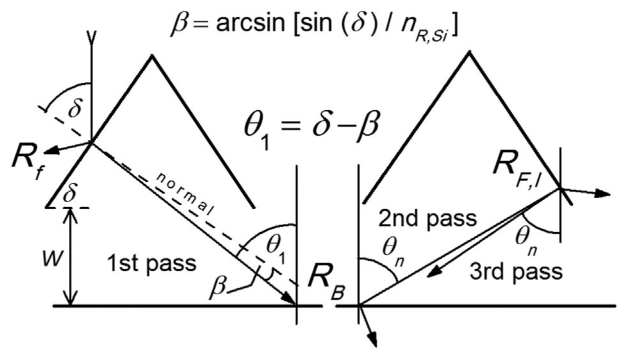

Figure 1. Sketch of the first optical passes of a light ray across a Si sheet with pyramidal front-surface texture of facet angle δ, where R_f is the front-surface external reflectance, R_{FI} is the front-surface internal reflectance, R_B is the rear-surface internal reflectance, and W is the thickness. In the sheet, $\theta = \theta_1$ at the first pass and $\theta = \theta_n$ at the second and successive optical passes. Pyramid dimensions are exaggerated. Relationships among internal angles are indicated, where $n_{R,Si}$ is the refractive index of Si.

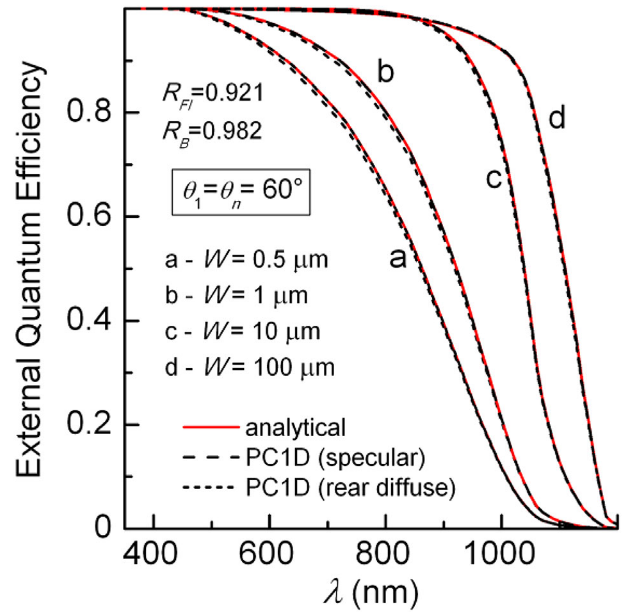

Figure 2. Analytical and numerical *EQE*-curves of solar cells having equal device, transport and optical parameters and different *W*-values. PC1D-curves are relevant to two settings of internal surfaces.

Concerning the third and subsequent passes of internal light across a given device, this model is such that, "because only weakly absorbed photons survive the first round trip of the device thickness, subsequent photogeneration resulting from these trapped photons is assumed to occur uniformly over the device thickness".[3] In thin devices, also non-weakly absorbed photons may survive the first round trip. In the case of thin devices, consequently, assuming uniform absorption after the first round trip of the device thickness is likely to underestimate light-generation.

3. Check and Correction Procedure

In **Figure 2**, curves of external quantum efficiency (*EQE*) as calculated with PC1D at both the settings for internal rear surface mentioned in the previous section are shown together with analytical *EQE*-curves calculated with the exact analytical expressions derived from the analytical solution to minority-carrier transport in uniformly doped regions,[5] which are reported in the appendix.

The curves in Figure 2 are relevant to cells having the structure and transport parameters listed in **Table 1** and various values of thickness, *W*. The internal reflectance of these cells is $R_{FI} = 0.921$ at the front and $R_B = 0.982$ at the back (see Figure 1). The cells have $R_f = 0$ at all λ-values (see Figure 1). Such devices have been already simulated elsewhere.[6,7] As can be seen, analytical exact and PC1D curves only overlap in the case, where, in PC1D, specular internal surfaces are imposed. The PC1D-curves calculated at diffuse rear surface are systematically lower than the remaining ones up to $W = 100\,\mu$m. We can so conclude that, as expected, the PC1D diffusion model underestimates light-generation in thin cells.

In **Figure 3**, the discrepancy ΔJ_{sc} between the values of short-circuit current density J_{sc}, calculated with PC1D at the two aforementioned settings is reported for *W* ranging from 0.06 to 300 μm. Since, in both settings for rear surface, the light-generation at the first optical pass is the same, ΔJ_{sc} only depends on the second and successive passes of trapped light. This observation allows making up a correction procedure for simulations performed with PC1D at $\theta_1 < 60°$ and $\theta_n = 60°$, which require imposing diffuse rear surface. In these cases, a previous determination of a ΔJ_{sc}-curve (or value) at $\theta_1 = \theta_n = 60°$ is necessary, to be added to the J_{sc}-curve (or value) calculated at $\theta_1 < 60°$, $\theta_n = 60°$, and diffuse rear surface. This removes the systematical underestimation of J_{sc} in thin devices, which is associated to assigning diffuse rear surface in PC1D. In the case of the cells simulated in the present work, the ΔJ_{sc}-curve to be added is shown in Figure 3.

4. Application

For the cells simulated in the present work, we have calculated with PC1D $J_{sc}(W)$-curves by using both the non-standard Lambertian model presented in Ref. [4], which we call "Green" from the name of its author, and a model, where $\theta_1 = 41.6°$ and $\theta_n = 60°$, which we call "quasi-standard" Lambertian model.

In the Green model, at all optical passes, $\theta = \theta_{op}$ is assigned with θ_{op} being a function of λ and *W* given by[4]

$$\theta_{op} = \cos^{-1}\left[\frac{1 + a(aW)^b}{2 + a(aW)^b}\right]$$

Table 1. Device and transport parameters of the modeled cells.

Region	Thickness (μm)	Doping density (cm^{-3})	Surface Recombination velocity ($cm\,s^{-1}$)	Diffusion length (μm)
Emitter	0.05	10^{19}	0	20
Base	W − 0.05	10^{16}	0	200

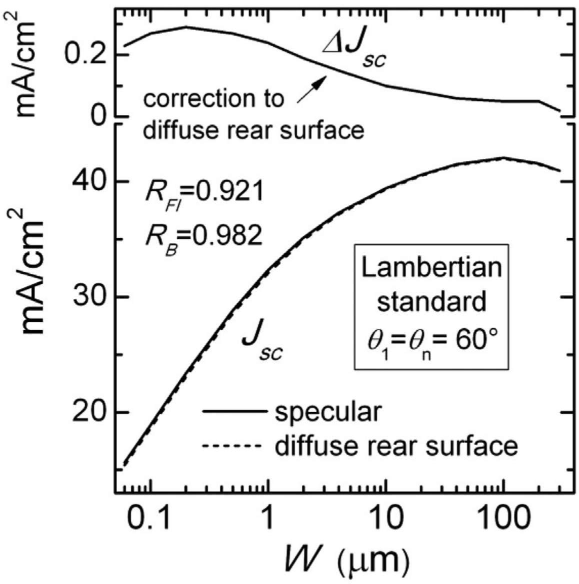

Figure 3. $J_{sc}(W)$-curves of solar cells having same device, transport and optical parameters as the cells in **Figure 2**. Curves are calculated with PC1D at two settings for internal surfaces. The discrepancy $\Delta J_{sc}(W)$ between curves is also reported.

where $a = 0.935$ and $b = 0.67$. The Green model assumes optically diffusive front surface [4] and can be easily implemented in PC1D at flat surfaces by assigning $\alpha/\cos\theta_{op}$ to absorption coefficient at each λ-value [6,7].

The quasi-standard model corresponds to a typical textured cell ($\delta = 54.74°$), where light is diffused at the rear surface so that standard Lambertian regimen only begins at the second optical pass. In the quasi-standard model, therefore, front surface is not optically diffusive.

The resulting $J_{sc}(W)$-curves are reported together with $\Delta J_{sc}(W)$-curves in **Figure 4**. In that figure, the curve relevant to the quasi-standard model is reported before ("diffuse" curve) and after ("corrected" curve) adding the correction-curve in Figure 3. As can be seen, the "Green" and "quasi-standard" models are practically equivalent in thin devices.

5. Discussion

As can be seen in Figure 3, the correction to J_{sc} due to the PC1D "diffusion model" is very small: it is of the order of 0.2 mA cm^{-2}, that is, no more than 1.5% of the total J_{sc}. It is a minor effect, which would probably be surmounted by other sources of uncertainty in real situations. However, removing the systematical underestimation of J_{sc}, which is associated to assigning diffuse rear surface in PC1D, could reveal helpful, if sources of uncertainty are of analogous or lower magnitude and/or a very high accuracy is required as is the case of the application in Figure 4.

6. Conclusions

A method to model standard Lambertian optics ($\theta = 60°$ at all λ-values) with PC1D in thin and ultrathin Si solar cells has been

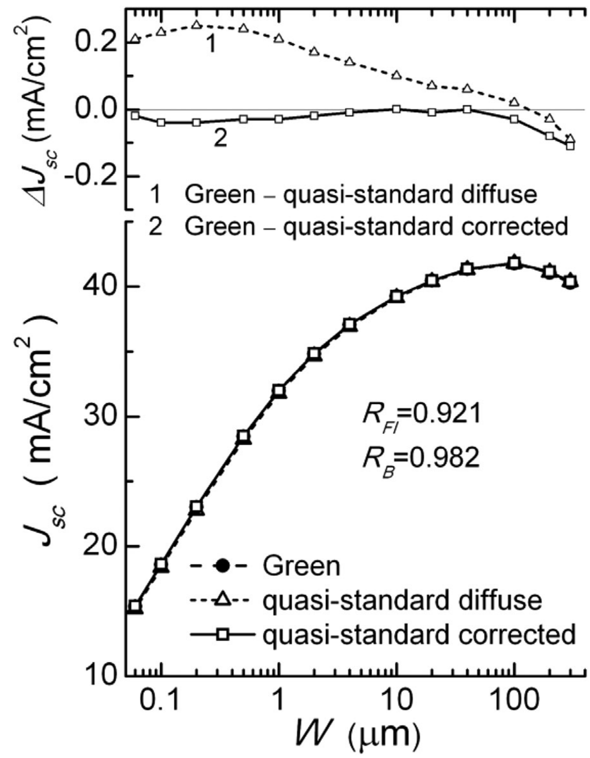

Figure 4. Comparison between Green and quasi-standard Lambertian models. $J_{sc}(W)$-curves are calculated with PC1D at same device, transport and optical parameters as used for the curves in Figures 2 and 3.

given. How to determine θ_1 has been explained. If $\theta_1 = \theta_n = 60°$, then specular internal surfaces must be imposed.

If $\theta_1 < 60°$ and $\theta_n = 60°$, then assigning diffuse rear surface is compulsory. In this case, a presented correction procedure must be applied.

An example of application of correction procedure has been given by showing that the "Green" model for Lambertian optics[4] and a "quasi-standard" Lambertian model, where standard Lambertian optics only begins at the second optical pass, are practically equivalent in thin devices.

Conflict of Interest

The author declares no conflict of interest.

Appendix

With the generation rate

$$g(x) = \frac{\alpha(1-R_F)}{\cos\theta} \times \frac{e^{-\frac{x\alpha}{\cos\theta}} + R_B T^2 e^{\frac{x\alpha}{\cos\theta}}}{1 - R_B R_{FI} T^2},$$

where α is the absorption coefficient and $T = \exp(-\alpha W/\cos\theta)$, and with $g'(x)$ being its first derivative, L the diffusion length, D the diffusivity, and S the surface recombination velocity for the relevant region, under the usual boundary conditions, the exact analytical solution to minority-carrier tranport in uniformly doped regions[5] gives the *EQE* contributions from emitter and base as

$$EQE_{em} = \frac{(1-\alpha^2L^2)^{-1}(1-R_{front})L^2}{\cosh(H_{em}/L)+(LS/D)\sinh(H_{em}/L)} \times \left\{ g'(x_{em})\left[\cosh\left(\frac{H_{em}}{L}\right)+\frac{LS}{D}\sinh\left(\frac{H_{em}}{L}\right)\right]+ -\frac{1}{L}\left[Lg'(x_0)-\frac{LS}{D}g(x_0)+g(x_{em})\times\left(\sinh\left(\frac{H_{em}}{L}\right)+\frac{LS}{D}\cosh\left(\frac{H_{em}}{L}\right)\right)\right]\right\}$$

and

$$EQE_{ba} = \frac{(1-\alpha^2L^2)^{-1}(1-R_{front})L^2}{\cosh(H_{ba}/L)+(LS/D)\sinh(H_{ba}/L)} \times \left\{ g'(x_{ba})\left[\cosh\left(\frac{H_{ba}}{L}\right)+\frac{LS}{D}\sinh\left(\frac{H_{ba}}{L}\right)\right]-\frac{1}{L}\left[g(x_{ba})+ -g(x_{ba})\left(1+\frac{LS}{D}\right)\exp\left(\frac{H_{ba}}{L}\right)-\left(Lg'(W)+\frac{LS}{D}g(W)\right)\right]\right\},$$

respectively, where x_0 is the emitter surface position, x_{em} the position of the interface between emitter, and space-charge region (SCR), H_{em} the emitter width, x_{ba} the SCR-base interface position, and H_{ba} the base width.

Keywords

light trapping, modeling and simulation, optical models, solar cells

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