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# DEVELOPMENT AND IMPLEMENTATION OF A REFINED MODEL FOR COMPREHENSIVE CHARACTERIZATION AND OPTIMIZATION OF HIGHLY EFFICIENT SILICON SOLAR CELLS

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ABSTRACT: Crystalline Silicon (c-Si) remains a dominant photovoltaics material in solar cell industry. Currently, scientific and technological advances make possible of producing the c-Si solar cells (SCs) efficiency close to the fundamental limit. Therefore, combining the experimental results with modeling becomes crucial to further improve the efficiency and reducing the photovoltaics systems cost. We carried out the experimental characterization of the highly-efficient textured c-Si SCs and compared the results with the analytical modeling formalism [1] and a *preliminary* modeling, using the commercial solar cell simulation software [2]. The analytical model accounts for all recombination mechanisms, including nonradiative exciton recombination and recombination in the space-charge region (SCR). To compare the theoretical results with the experiment, we proposed empirical formula for the external quantum efficiency (EQE), which describes its experimental spectral dependence near the absorption edge. The approach used allows a comparative modeling of the short-circuit current and photoconversion efficiency in the textured crystalline silicon solar cells. The theoretical results, both from analytical formalism and computational tools, compared to the experimental measurements, allowed: (i) Validating the formalism developed, which was then used to optimize the key parameters of the SCs, such as the base thickness, doping level and others. (ii) We demonstrated several advantages of the application of our analytical formalism, compared to the computational software tools.
Keywords: silicon, solar cell, texture, efficiency, recombinations, optimization

## 1 INTRODUCTION

To reduce the cost of solar cells (SCs) while maximizing their photoconversion efficiency $\eta$, surface texturing is used to reduce the optical reflection losses and maximize the number of photoactive photons absorbed. Therefore, surface texturing in photovoltaics systems is currently drawing much attention [3-5]. Recent record-breaking efficiency of 26.6% for Si solar cells have been achieved on such textured systems [6-8], while the theoretical limit of the efficiency for Si SCs is about 29%. The important component of the photon management is the texturing, an artificial roughening of the surface, which reduces its reflection by increasing the chances for reflected light bouncing back onto the semiconductor surface, rather than out of it to the surrounding and increasing the photon propagation path inside the semiconductor. This is important for making the solar cells thinner and even flexible [5], [9]. The commonly accepted model for the textured surface from the reflection reduction point of view is a completely randomized Lambert surface [10], although different textured patterns are experimentally used [5]. This complicates the theoretical, both analytical and computational, descriptions of the textured SCs.

To advance even more in improvement of the SCs efficiency the available optimisation approaches should be further developed and applied. Currently, further increase of the silicon SC efficiency becomes more and more difficult, and requires better consideration of the physical processes in the SCs. In particular, to further increase the SCs efficiency it is necessary to take into account all contributing recombination mechanisms in silicon. This has to include a non-radiative exciton recombination via deep impurity centers [11] and recombination in the space-charge region (SCR) [12] . Still, the above two mechanisms are not included in the existing SC optimization formalisms and software [2]. However, as we previously demonstrated [13], these recombination processes are detrimental in the high-efficiency silicon-based SCs. They may significantly influence the SCs efficiency as compared to the mechanisms that are already considered, such as, in particular, the radiative and band-to-band Auger recombinations. In order to model and optimize textured high-efficiency silicon SCs we first measured and analyzed experimentally the external quantum efficiency (EQE). For the analytical formalism the main input parameter required is the experimentally measured short-circuit current density $J_{SC}$. Next, the short-circuit current and the photoconversion efficiency under AM1.5 conditions, both dependent on the base thickness $d$ and its doping level are derived, and used to optimize the characteristics of the textured silicon SCs. Important is that the theoretical approach, presented here, is applicable to any type of textured SCs surface: The experimentally measured short-circuit current density $J_{SC}$ is a required parameter in the analytical formalism [1]. Apart from being dependent on the standard solar cell parameters such as recombination, doping level, etc., $J_{SC}$ also includes implicitly influence of the surface texture type, antireflective coating (ARC), and angular distribution of the photoactive photon flux in the semiconductor. The last three factors cannot be very accurately accounted for in the solar cell simulations software.

As an example, to demonstrate a considerable variation of the SC reflectivity, we used the online simulator Opal 2 [14] to calculate the change in the Si solar cell reflectivity when the texture was created using regular pyramids, random pyramids and spherical caps, as well as the planar surface. The results are shown in Fig. 1. For this example, we also used a single layer $TiO_2$ ARC with thickness of 78 nm (the technical details of the

reflectivity calculations are discussed in the next sections)

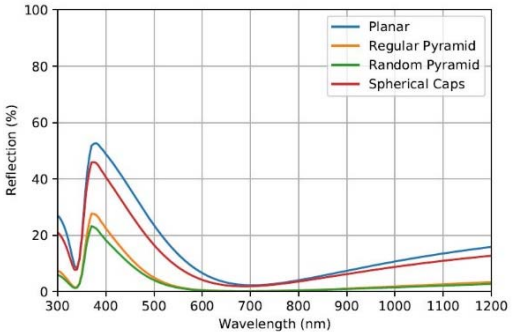


**Figure 1**: Calculated silicon solar cell surface reflectivity under AM1.5 illumination for different texture types *vs*. flat (planar) surface: regular pyramids (orange line), random pyramids (green) and spherical caps (red) *vs*. planar (blue)). The single 78 nm thick layer $TiO_2$ ARC has been used. Texturing combined with ARC substantially lower the reflectivity losses in SCs.

Using the solar cell simulation Quokka software [2] we also optimized the solar cells considered, the preliminary results of the simulation are presented and compared to the experimental results as well as the analytical formalism outcome.

To develop the analytical formalism, it is established that the experimental spectral dependencies of the external quantum efficiency $EQE(\lambda)$ in textured silicon SCs near the absorption edge can be described by an empirical formula $EQE(\lambda)=[1+b/(4n_r(\lambda)^2\cdot\alpha(\lambda)d)]^{-1}$, where $\alpha(\lambda)$ is the light absorption coefficient, $d$ is the base thickness, $n_r$ is the refractive index, and $b$ is a non-dimensional coefficient, which characterizes the texturing profile impact. It is usually greater than 1, however, when $b$=1 the empirical formula transforms into the well-known Yablonovitch formula [15]. Physical meaning of the parameter $b$ is the ratio of the photon path length in the case of a perfectly randomized surface, considered in [10], to the photon path length in a particular sample with nonrandomized flat surface. This formula allows to analytically model and optimize the photo-conversion efficiency of the solar cell in terms of base thickness $d$.

For the textured silicon SCs considered, the experimental *EQE(λ)* dependence was compared to both empirical and simulated dependencies. It is shown that close to the absorption edge *EQE(λ)* behavior can be accurately described by the empirical formula with the parameter *b,* ranging from 1.6 to 4. Using the experimental values *EQE(λ)* and the proposed formula, we calculated the dependence of the short-circuit current density $J_{SC}$ on the base thickness $d$ for the textured SCs.

## 2 SUMMARY OF THE ANALYTICAL FORMALISM

We model the silicon $p^+$- $n$ - $n^+$ type SCs, for details of the analytical formalism [1]. When the bulk minority-carriers diffusion length $L_d = \sqrt{D_p \tau_{eff}}$ is much bigger than $d$/4 ($d$ is the base width), and combined surface and SCR recombination velocity $S_{SC} + S_{S0} << \frac{2D_p}{d}$, the excess carriers' concentration is practically uniform in the base region. (Here $D_p$ is the carriers' diffusion coefficient and $\tau_{eff}$ is their effective recombination time). In this case within the narrow-base approximation the *I-V* characteristic under the illumination can be written as:

$$I(V) = I_L - I_r(V) + \frac{V+IR_s}{R_{SH}}, \quad (1)$$

where the first term is the photocurrent, the second term is the recombination current, $A_{SC}$ is the SC area, and $R_S$ and $R_{SH}$ are its series and shunt resistances. The excess carrier concentration depends on the applied voltage $V$ by a modified law of mass action as:

$$(n_0 + \Delta n)(p_0 + \Delta n) = n_{i0}^2 \, exp\left(\frac{\Delta E_g + q(V-IR_S)}{kT}\right), \quad (2)$$

where $n_{i0}$ is the intrinsic concentration at low injection level [7], and $\Delta E_g(n_0, \Delta n)$ is the bandgap narrowing in Si [8]. Eq. (2) can be used to write the excess concentration as:

$$\Delta n = -\frac{n_0}{2} + \sqrt{\frac{n_0^2}{4} + n_{i0}^2 e^{\Delta E_g/kT}(e^{q(V-IR_s)/kT} - 1)}. \quad (3)$$

Equations (1) – (3) have to be solved numerically. The open-circuit voltage and the short-circuit current are obtained by setting in (1) $I$ and $V$ to zero, respectively. The expression for $V_{OC}(V)$, obtained from (3) has the following form:

$$V_{OC} = \frac{kT}{q} ln\left(\frac{\left(\Delta n_{OC}+\frac{n_0}{2}\right)^2 - \frac{n_0^2}{4}}{n_{i0}(T)^2 e^{\Delta Eg/kT}} + 1\right). \quad (4)$$

The excess electron density $\Delta n_{OC}$ at open-circuit conditions when $L_d >> d$, can be found from the balance equation in the form:

$$I_L/q = A_{SC}\left[\frac{d}{\tau_{eff}(\Delta n_{OC})}\right]\Delta n_{OC}, \quad (5)$$

where the effective recombination time $\tau_{eff}(\Delta n_{OC})$ is determined by expression (6). The total effective recombination time in the SC depends on the intrinsic mechanisms (that cannot be decreases below the well-defined fundamental limits) and extrinsic recombination mechanisms (that can be modified, *e.g.*, in the process of the sample preparation, *etc*.)

$$\tau_{eff}^{-1} = \tau_{intr}^{-1} + \tau_{extr}^{-1}, \quad (6)$$

with the lifetime for intrinsic recombination, which includes radiative and interband Auger recombinations:

$$\tau_{intr} = \left({\tau_{rad}}^{-1} + {\tau_{Auger}}^{-1}\right)^{-1}. \quad (7)$$

The extrinsic recombination lifetime (which can be reduced by sample bulk preparation, surface passivation, etc.) depends on Shockley-Reed-Hall lifetime, non-radiative exciton recombination lifetime due to Auger mechanism (recombination via deep level [5]), lifetime due to surface recombination and lifetime for recombination in the SCR [6]. In general

$$\tau_{extr} = \left(\tau_{SRH}^{-1} + (\tau_{exc}^{n})^{-1} + \left(\tau_{eff}^{s}\right)^{-1} + (\tau_{scr})^{-1}\right)^{-1}. \quad (8)$$

The photoconversion efficiency $\eta$, photovoltage $V_m$,

photo-current $I_m$, and output power $P_m$ in the maximum-power output regime are found by setting the derivative of $P = IV$ with respect to the voltage to zero.

This self-consistent approach for textured Si solar cells efficiency $\eta$ optimization has been applied and validated experimentally. Dark and light *I–V* characteristics as well as light intensity dependence of the open-circuit voltage were measured for a number of highly efficient silicon *p-n* junction SCs with the photoconversion efficiency $\eta \geq 20\%$. The spectral dependencies of $EQE(\lambda)$ under AM1.5 conditions were also investigated experimentally.

## 3 NUMERICAL SIMULATIONS

For the numerical simulations we considered c-Si solar cells with both the planar and top surfaces The top surface reflection was calculated using the SunSolve Software provided by PV Lighthouse [14], as was shown in Fig, 1. In this simulation, a 78 nm thick $TiO_2$ ARC film was deposited on top of a 500 μm silicon substrate [16]. The first simulation uses a film with a planar texture and the minimum reflection is 2.2% at 705 nm. The second simulation uses a film with a regular upright pyramid texture with a characteristic angle of 54.74° and has a minimum reflection of 0.2% at 690 nm. The third simulation uses a film with a random upright pyramid texture with a characteristic angle of 54.74° and has a minimum reflection of 0.2% at 685 nm. The last simulation uses a film with a spherical cap texture with a characteristic angle of 54.74° and has a minimum reflection of 1.8% at 690 nm.

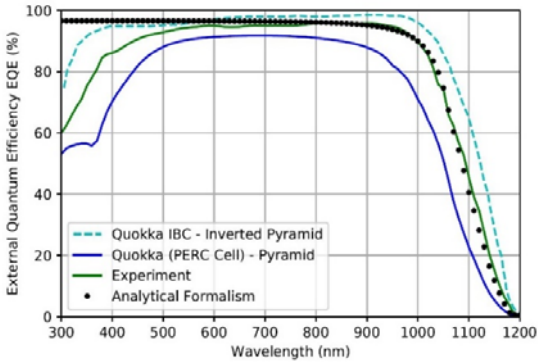


**Figure 2**: Experimental $EQE(\lambda)$ for commercial 21.3% efficient SunPower SC (green line). Black circles are for *EQE* using empirical formula [1]. Cyan-dashed line is the calculated $EQE(\lambda)$ dependence for the 25.6% efficient IBC SC [17], and, for comparison, the blue line is for the PERC solar cell.

Preliminary simulations of *EQE*, *I–V* characteristics, and the efficiency were carried out using the Quokka 2 software with the *standard* parameter set from [17], including the bulk recombination parameters, for Auger bulk recombination, the radiative recombination, etc. The External Quantum Efficiency was calculated using a thickness of 165 μm and a doping level of $9 \cdot 10^{14}$ cm$^{-3}$. The IBC external quantum efficiency was obtained from [4]. For figure 3, we calculate the *I–V* current density as a function of voltage using a thickness of 165 μm and a doping level of $9 \cdot 10^{14}$ cm$^{-3}$.

## 4 COMPARISON: THEORY *VS.* EXPERIMENT

In Fig. 2 we present the photon wave length dependent external quantum efficiency $EQE(\lambda)$. This compares the experimentally measured and theoretical results, calculated using the empirical formula [1], as well as simulated using Quokka software. The EQE for 25.6% efficient IBC SC is from [17], and that one from the PERC solar cell, for comparison.

Next Fig. 3 compare the measured and calculated light *I–V* characteristics. Circles are the experimental values for the commercial 21.3% efficient SunPower SC. The solid lines are from the theory: the red line is from the analytical formalism [1]; green line is from Quokka simulations for the IBC SCs.

As can be seen from Figs. 2 and 3, the analytical formalism [1] provides very good agreement with the experimentally measured results. The agreement between the preliminary Quokka 2 simulations with the experiment, however, is not as good for the analytical formalism

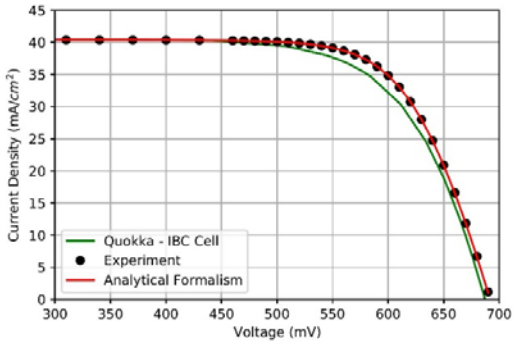


**Figure 3**. Measured (circles) and calculated (line) light *I–V* characteristics. Circles are the experimental values for the commercial 21.3% efficient SunPower SC. The solid lines are from the theory: the red line is from the analytical formalism; green line is from Quokka simulations for the IBC SC.

As it is clear from Figure 3, the open circuit voltage $V_{OC}$, calculated using both theoretical approaches are in a perfect agreement with the experimental results, while below $V_{OC}$ the simulated (using Quokka) current deviates from the experimental values. We attribute, however, the disagreement with the experiment mostly due to the use of the standard [17] parameter set in the Quokka input, especially series and shunt resistance. In the future simulations the focus will be on the optimization of series and shunt resistances as well as other parameters.

## 5 CONCLUSIONS

We compared the results of the comprehensive analytical formalism [1] that models and optimizes the high-efficiency textured silicon-based solar cells with the experimental characterization and the *preliminary* results from the numerical simulation software Quokka 2 [2]. It is demonstrated in [1] that the contribution of nonradiative exciton recombination, as a rule, exceeds the radiative recombination contribution and substantially affects the photo-conversion efficiency, stronger than the gap narrowing effect. Such important mechanism, however,

cannot be readily modelled within the numerical simulation software.

The calculated SCs parameters such as the short-circuit current density $J_{SC}$, open-circuit voltage $V_{OC}$ and photo-conversion efficiency $\eta$ have been determined for several SCs types. Following [1], a very good agreements of the calculated characteristics with experimental ones has been achieved, better than using Quokka 2 [2] simulation. We believe that using the accurate and specific, to the SC considered, parameter sets will allow better agreement of the simulation and the experiment. Using the analytical formalism [1] allows to optimize the SCs base thickness and the base doping level. Further Quokka 2 modeling is in progress.

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