**Characterization and optimization features of high-efficiency silicon solar cells with dominating surface recombination**

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**Abstract.** This work establishes the features of modeling photoconversion processes in highly efficient solar cells based on single-crystal silicon for the case when the contribution of surface recombination significantly outweighs the contributions of recombination in the space charge region (SCR) and non-radiative excitonic recombination with the participation of impurity centers. It is shown that in this case the key characteristics of the photoconversion process, namely the dark and light current-voltage characteristics and the dependences of the output power of SС, obtained with and without taking into account recombination in the SCR and non-radiative excitonic recombination with the participation of impurity centers, practically coincide with each other.

The modeling results were compared with the experiment for the SС from two works, in which the above-mentioned conditions took place. The analysis confirmed the consistency of the theoretical dependences obtained with and without taking into account the recombination in the SCR and non-radiative exciton recombination with the experiment. It is shown that optimization of the base doping level and thickness of the considered SC allows to increase its efficiency from 24.37% to 24.62%.

The results obtained in this work allow to explain why previously the recombination in the SCR was not taken into account in the theoretical modeling of the characteristics of the SС based on single-crystal silicon in the overwhelming number of works, and also to show that the general approach is valid in the case of any ratio between the components of the recombination currents in single-crystal silicon.

**Keywords:** modeling, silicon solar cell, surface recombination rate, recombination in the SCR, photoconversion efficiency.

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**Introduction**

The reviews [1-4] analyzed the state of research and prospects for photovoltaic applications. The dominant role in these research and development today is played by highly efficient solar cells (SCs) based on monocrystalline silicon, in particular, their share in production reaches 97% [5].

Since the record efficiency of silicon SCs is 27.3% [6] and has closely approached the theoretical limit of ~29.6% [7-9], the importance of using adequate model representations for accurate simulation and optimization of their characteristics is increasing. In [10], a theoretical approach was developed that allows for correct modeling of the experimental dependences of the key photovoltaic characteristics of the mentioned SCs. This approach takes into account the following recombination mechanisms in monocrystalline silicon. These are radiative recombination, interband Auger recombination, surface recombination, bulk Shockley-Reed-Hall recombination, space charge region (SCR) recombination, and non-radiative excitonic recombination by the Auger mechanism via deep impurity level. The last two mechanisms are not taken into account in existing works on modeling the characteristics of silicon SCs, with the exception of our previous works. This work provides an explanation of when this can be done. The specified neglect is valid when the SCR recombination and non-radiative excitonic recombination are significantly smaller than the surface recombination.

In this work, we first theoretically modeled the key photoelectric and optical characteristics for the SCs obtained in [11]. The SCs developed in this work are designed according to the so-called IBC scheme with back contacts and separating p+-n and isotype n-n+ barriers.

The modeling approach developed in [10] was used for their modeling characterization. The analysis was performed using six and four-recombination processes describing recombination in the SC base region. In four processes, Shockley-Reed-Hall (SRH) recombination, surface recombination, interband Auger recombination, and radiative recombination mechanisms were taken into account. When considering six processes, recombination in the SCR and non-radiative excitonic recombination by the impurity Auger mechanism were additionally taken into account.

It was shown in [10] that when the recombination in the SCR exceeds the surface recombination [12-16], the approximation of six recombination processes better describes the experimental characteristics of the SC than the approximation of four recombination processes. Particularly large differences in these cases are observed when calculating the excess concentration of electron-hole pairs dependent effective lifetime in the base region. In the SCs that we analyzed in this paper, it turned out that the surface recombination significantly exceeds the recombination in the SCR. Therefore, both approximations give the same result, as will be shown below.

Another feature revealed in the analysis of the experimental results obtained in [11] is a weaker-than-usual dependence of the surface recombination rate *S*(Δ*n*) on the excess concentration of electron-hole pairs. In the general case the rate can be described as:

, (1)

Where *S*0 is the initial surface recombination rate, *n*0 is the equilibrium electron concentration in the base, and *r* is the slope of the *S*(Δ*n*) dependence. Usually, for most silicon SCs, the value *r* is 1, but in this case *r* = 0.62. As will be shown below, a value less than 1 *r* is realized in the case when the charge in the SCR of the *n*+ layer of the isotype *n - n*+ junctions is small compared to the charge of the *p*+ area.

It should be noted that despite the sufficiently high surface recombination rate, the efficiency of 24.37% in this SC is quite high. One reason for this is the small charge value of the SCR of the n+-region; because of this, the surface recombination rate at the maximum power point (MPP) is smaller than in the case of *r* =1.

The second reason is the efficient light capture due to high-quality front surface texturing, as evidenced by the *EQE (λ)* dependences and high short-circuit current density (41.95 mA/ cm2). All of the above compensate for the relatively small open-circuit voltage.

Finally, we calculated the light *J–V* characteristics and the dependences of the output power *P* on the applied voltage, experimentally obtained in [17], in the approximations of six and four-recombination mechanisms and made sure that they also visually coincide. We have already calculated the light *J–V* characteristics obtained in [17], in the approximation of six recombination mechanisms. The calculation results were published in our work [18], but the calculation in the approximation of four recombination mechanisms was not carried out. It should be noted that [17] was published earlier than [11] and it considered the SCs with flat surfaces. Both works were carried out by the same research group. The main goal was to analyze the wavelength-dependent External Quantum Efficiency *EQE(λ)* and Internal Quantum Efficiency *IQE(λ)* for a flat SC with a flat surface in the general and limiting cases of large diffusion lengths compared to the thickness of the base. We derived the corresponding expressions in [18] and established that the aforementioned limiting case of large diffusion lengths compared to the substrate thickness is appeared in [17]. We calculated the recombination rate in the SCR when the inverse lifetime in the SCR is described by a Gaussian. This part of the work is based on the theoretical approach proposed in [18]. The work is structured so that we first interpret the results obtained in [11], and only then analyze the experimental light *J–V* characteristics and the applied voltage dependent output power, obtained in [17] in the approximation of six- and four-recombination mechanisms.

**2. Calculation of external quantum yield and short circuit current**

In [10], a theoretical approach is described that allows modeling the short circuit current *JSC*, having dependencies for *EQE*(*λ*) in the device structure. Its essence is as follows. As our analysis of the experimental dependence of *EQE*(λ) in SC samples of different thicknesses [15,19] has shown, it can be divided into two regions. In the first, short-wave region λ < 800 nm, which is denoted by the index s, the external quantum efficiency *EQEs*(λ) is practically independent of the sample thickness d. In the second, long-wave region, *EQE*l(λ) (λ > 800 nm), which is denoted by the index l, such a dependence is present. In the long-wavelength region near the absorption edge, the Lambertian is used to calculate the external quantum efficiency in the following form

 , (2)

where the fitting non-dimensional parameter *b* determines the shape of the *EQEl* dependence, and has the physical meaning of the ratio of the photon mean path length in an SC with ideal Lambertian surfaces to its actual mean photon path length, *n*Si is the refraction index and α(λ) is the absorption coefficient of silicon, *d* is the SC thickness. The parameter *f* is chosen so that the values of *EQEs* and *EQEl* coincide at λ = 800 nm.  Note that in the case when *b* = *f* = 1, expression (1) turns into the well-known formula for the absorption capacity of the SC, introduced in [20]. In the region λ < 800 nm, the experimental *EQEs*(λ) does not depend on the base thickness and is determined only by the losses due to reflection, shadowing, and absorption of light outside the base SC region.

By breaking the value *EQE*(λ) into two components, we can calculate the dependence *Jsc*(*d,b*):

 (3)

Here *I*(λ) is the spectral density of the photon flux under AM1.5 conditions.

Fig. 1 shows the experimental dependences of the external quantum efficiency SC obtained in [11]. As can be seen from the comparison of theory with experiment, they agree with each other at *b* =2.6 and *f* =0.973.



Fig. 1. Experimental spectral dependencies of the external quantum efficiency *EQE*(λ) of IBC SC, obtained in [11] (points), while the solid line is the calculation according to formula (2).

Using the expressions (2) and (3), we calculated the dependence of the short-circuit current of the SC from work [11] on the base thickness *d*, as shown in Fig. 2.



Fig. 2. Calculated dependence of the short-circuit current density on the base thickness *d* for IBC SC, developed in [11].

3. **Dependences of the effective lifetime on excess concentration**

We will describe below the algorithm for finding the experimental values ​​of the total recombination rate in the SCR, namely, the values ​​of the recombination rate in the SCR *SSCR* and in the part of the SCR that became neutral due to the reduction of the bands bending upon illumination, as proposed in [11]. The experimental  value is found using the expression:

 , (4)

where *d* is the SC base thickness,  is an effective lifetime without the component describing the recombination time in the SCR. This effective lifetime can be found from the following expression:

, (5)

where τ*SRH* is the SRH recombination lifetime, τ*ex* is the non-radiative exciton recombination lifetime, τ*S* is the surface recombination lifetime, τ*Auger* is the interband Auger recombination lifetime and τ*rad* is the radiative recombination lifetime.

The theoretical value  is found from the expression

 , (6)

where

, (7)

. (8)

. (9)

Here, τ*R* is the lifetime in the SCR, *br*= *Cps/Cns*, *Cps*, *Cns* is the coefficients of hole and electron capture by the recombination center, respectively, *y* is the dimensionless potential, *ni* is the concentration of intrinsic charge carriers, *Et* is the energy of the recombination center, *T* is the temperature, *w* is the thickness of the SCR,  is Debye length, *q* is the elementary charge, *k* is the Boltzmann constant, ε0, εSi is the permittivity of free space and relative permittivity of silicon, respectively, *y*0 is the non-equilibrium non-dimensional band bending value on the surface of the weakly doped region, which depends on the injection level Δ*n* and is found from the integral neutrality condition, and *yw* is the non-equilibrium non-dimensional potential on the boundary between the SCR and the quasi‑neutral region.

Fig. 3 shows the experimental dependence of the recombination rate in the SCR (dots) and its theoretical fit in blue.



Fig. 3. Recombination rate in SCR as a function of excess concentration. Experiment for SC from [11] (points) and the correlated theoretical fit (solid line).



Fig. 4. The excess concentration dependent effective lifetime in the SC base: experiment from [11] (solid circles) and the theoretical (lines). The solid blue line is calculated in the presence of recombination in the SCR, while the dashed curve is for the recombination in the SCR absent.

Fig. 4 shows the experimental dependence of the effective lifetime in the SC base, as measured in [11], and our similar theoretical dependences. Having found the recombination rate in the SCR, we can now calculate the theoretical dependence of the effective lifetime on the excess concentration, which is shown in Fig. 4 (solid curve). In the case when the recombination rate in the SCR is negligibly small, the dependence of the effective lifetime on the excess concentration is described by the dashed curve shown in Fig. 4. Comparing the last two curves, we can see that in this case the largest difference between them in the region of their maximum values is of the order of 9%, if the value Δ*n* is 1.3∙1014 cm-3 and 15%, when Δ*n* = 1.7∙1013 cm-3. These values are significantly smaller than the difference between the effective lifetime in the presence and absence of recombination in the SCR, obtained in [11]. This is because the recombination rate in the SCR in this case in the region of actual excess concentration values is more than an order of magnitude smaller than the surface recombination rate, and in [11], the recombination in the SCR is higher than the surface one. This means that in this SC, the recombination in the SCR plays a significantly smaller role than in the SCs considered in [11].

Note that the agreement between experimental and theoretical dependence for the effective lifetime in the base (Fig. 4) was obtained when using the coefficient *r* = 0.62 (see equation (1)). The introduction explained that this is possible if the charge in the isotype junction is significantly smaller than in the anisotype junction.

Let's prove it. The neutrality equation for the isotype junction is the following:

, (10)

where is the surface charge density in the isotype junction. In this case, *N* is negative.

 

Fig. 5. Dependences of the surface recombination rate *S* on the excess concentration at the interface between the n and n+ regions of the SC according Eq. (1) (points) and Eq. (11) (red line) when the charge in the n+ region *N* =­ −0.515∙1011 cm-2 and the parameter *r* = 0.62 (a) and when the charge in the n+ region *N* =­ −1012 cm-2 and the parameter *r* = 1 (b).

Fig. 5 shows the dependences of the surface recombination rate for the case when such recombination occurs through a discrete trap level located near the middle of the band gap at the boundary of the *n* and *n*+ regions (defect-assisted SRH recombination). The expression for this recombination rate has the following form:

 , (11)

with *S*00 = 1/*CpsNts*, where *Cps*is the hole capture coefficient, *Nts* is the surface defects level concentration, *br*= *Cps/Cns*, and *Cns* is the electron capture coefficient.

In the case when *N* =-0.515∙1011 cm-2, dependence (11) is in satisfactory agreement with (1) at *r* = 0.62 (see Fig. 5a). If *N* = -1012 cm-2, then the coefficient *r* in the dependence *S*(Δ*n*)equals 1 (see Fig. 5b).

4. **Modeling of light *J-V* characteristics and dependencies of power on applied voltage for SC of work** [11]



Fig. 6. Light *J*(*V*) and *P*(*V*) characteristics SC from [11]. Points are experiments, and lines (1-3, 4-6) are the theoretical dependences calculated respectfully using six-, five-, and four-recombination mechanisms. Lines 1-3 and 4-6 visually coincide.

Fig. 6 shows the experimental dependencies for light current density-voltage *J–V* characteristics obtained in [11]. Theoretically, the light current-voltage characteristic for silicon SCs can be determined from expressions (12)-(15):

, (12)

, (13)

, (14)

, (15)

where *JL*(*V*) = *IL*(*V*)/*ASC* is the total current density, *ASC* is the SC area, *JSC* is the short-circuit current density, *Jr*(*V*) is the recombination (dark) current density, *V* is applied voltage, *RS* and *RSH* are series and shunt resistance, *n* = *n*0 + Δ*n* is the total electron concentration in the neutral volume of the base and Δ*Eg* is the temperature-dependent narrowing of the semiconductor band gap.

Fig. 6 also shows theoretical dependencies for light *J–V* characteristics, calculated using approximations of six, five, and four recombination mechanisms. The meaning of the six- and four- mechanism approximations is described above. The case of five mechanisms corresponds to neglecting the recombination in the SCR and taking into account non-radiative exciton recombination. The theoretical dependencies, shown in Fig. 6, as well as in Fig. 7, were simulated in the following order. First, the dependences were constructed to approximate six recombination parameters, then five and, finally, four recombination parameters. As can be seen from Fig. 6, the obtained dependencies visually coincide with each other and are consistent with the experiment. In the case of six-recombination approximation the following parameters were used: *S* =14.57 cm/s, *RS*=0.165 Ohm∙cm2, τ*SRH*=7∙10-3 c, *r* =0.62 , τ*R* =7∙10-5 c , *br* =0.1, *RSH*=3∙104 Ohm∙cm2, and *JSC*=41.95 mA/cm2. In the case of five recombination mechanisms, only the surface recombination rate and the series resistance are changed, that is *S* =14.77cm/s, and *RS*=0.183 Ohm∙cm2. When only four mechanisms are considered, the surface recombination rate and series resistance equal *S* =16.1 cm/s, and *RS*=0.15 Ohm∙cm2.

The dependence of the SC output power on the applied voltage is described by the expression

. ( 20 )

Fig. 6 also shows the experimental and theoretical dependences *P*(*V*) calculated in the approximations of six, five, and four recombination mechanisms, using the above parameter values. As in the case of light *J-V* characteristics, they coincide with each other. The reason for their coincidence is the insignificance of the recombination in the SCR and non-radiative exciton recombination compared to the surface recombination rate.

The expression for the dark current has the following form:

 . (16)

. (17)

Finally, the dependences of the short-circuit current on the open-circuit voltage are determined from the equations

, (18)

. (19)

Fig. 7 shows the theoretical dependences for the dark current on the applied voltage and the short-circuit current on the open-circuit voltage in the approximations of four, five, and six recombination mechanisms. In this case, first, theoretical dependences for the dark *J-V* characteristics were calculated and plotted, and then theoretical dependences *JSC*(*VOC*)*.* In this case, the shunt resistance is relatively small (3∙104 Ohm∙cm2), and the surface recombination rate significantly exceeds the recombination rate in the SCR and the rate of non-radiative exciton recombination. In this case, all the calculated and plotted curves practically coincide visually.



Fig. 7. Theoretical dark *J–V* characteristics (lines 1 - 3) and dependencies *JSC*(*VOC*) (lines 4 - 6), calculated using six (1,4,7,10), five (2,5,8,11) and four (3,6,9,12) recombination mechanisms for the case when the shunt resistance is 3∙104 (lines 1-6) and 3∙1010 Ohm∙cm2 (lines 7-12). Upper curve contains visually matching lines 1-6, while the middle and lower curves contains similarly matching lines 7, 10 and 8, 9, 11, 12 respectively.

The close similarity of the dark *J-V* characteristics and the short-circuit current dependences in this case is associated with the small series resistance and the limit of the maximum applied voltage and open-circuit voltage, while the shunt resistance is sufficiently small. It should be noted that with and without the recombination in the SCR, the dependencies coincide at both low applied voltages and open-circuit voltages only because, in the region of low voltages, the dark current is determined by the shunt resistance. If the shunt resistance is set to be large (about 1010 Ohm∙cm2 or more), then the dark current and the *JSC*(*VOC*) dependences in the presence and absence of recombination in the SCR differ (see Fig. 7). In this case, as before, theoretical dependences for the dark *J-V* characteristics were first calculated and plotted, and then theoretical dependences *JSC*(*VOC*).

Consider that most of the simulation programs for calculating key parameters of silicon-based SCs were developed before researchers learned to effectively minimize surface recombination. Therefore, it becomes clear why the theoretical dependencies obtained in the approximation of four recombination mechanisms were in good agreement with the experiment. The situation changed when technologies were developed for effective passivation of the surface of silicon crystals, which reduced the surface recombination to a few cm/s or even less [12, 21-25]. As the results of our studies, in particular in [10, 27], have shown, in cases where surface recombination is less than recombination in the SCR, taking the latter one into account is absolutely necessary. In this case, recombination in the SCR has a particularly strong influence on the dependence of the effective lifetime on excess concentration.

**5. Optimization of the parameters of the SC studied in [11]**

As in the case described in [10], the efficiency obtained in [11] can be increased by optimizing the base thickness and the base doping level. Our calculations showed that the maximum efficiency of 24.62% can be achieved at the base doping level of 5∙1015 cm-3 and the base thickness of 520 μm. The dependence of the output power of the optimized SC on the applied voltage for this case is shown in Fig. 8. Considering that the experimental efficiency from [11] was 24.37 %, the authors of the work outstandingly selected parameters that allowed getting the efficiency close to the optimal one.



Fig. 8. Theoretical light *J*(*V*) and *P*(*V*) characteristics of the optimized SC, calculated using the six recombination mechanisms approach.



Fig. 9. Dependence of the efficiency of SC photoconversion on the rate of surface recombination at the boundary of the isotype junction calculated using approaches with four (curve 1) and six (curve 2) recombination mechanisms.

Fig. 9 plots the dependencies of the photoconversion efficiency on the surface recombination rate, from which it can be seen that at *S* ≥ 20 cm /s, the values of the photoconversion efficiency calculated in the approximations of six and four recombination mechanisms visually coincide. It is also seen that even at *S* = 100 cm/s, the photoconversion efficiency remains sufficiently high.

6. **Modeling of light *I-V* characteristics and dependences of useful power on excess concentration for work** [17]



Fig. 10. Light *J*(*V*) and *P*(*V*) characteristics of the SC from [17]. Points are experiments, and lines are the theoretical dependences calculated respectfully using six (lines 1,3), and four (lines 2,4) recombination mechanisms. Lines 1,2 and 3,4 visually coincide.

Fig. 10 shows the experimental dependences for the light *J–V* characteristics from [17], as well as the theoretical ones in the approximations of six and four recombination mechanisms. The calculated graphs are using the formalism from [18] with the following parameters: τ*m* =3.8·10-6 s, *xm*= 8.5·10-6 см, σ =2.4·10-6 см, *br* = 0.1, τ*SRH* = 2.1·10-3 s, *S0* = 17.4 cm /s, *RS* =0.64 Ohm·cm 2, where τ*m* is the lifetime at the maximum point, *xm* is the position of the maximum, and σ is the dispersion of Gauss distribution.

As can be seen from the figure, the voltage-dependent light *J*(*V*) characteristics, calculated in the approximations of six and four mechanisms, visually coincide.

Fig. 10 also shows the experimental dependence of the output power on the applied voltage *P*(*V*) and the theoretical dependences in the approximations of six and four recombination mechanisms, calculated following the approach of [18]. As can be seen from the figure, the theoretical dependences of the output power, calculated in the approximations of six and four recombination mechanisms, also coincide.

In this case, the excess concentration at the maximum efficiency point is 1.96∙1014 cm-3, *S* =18.1 cm/s, *SSCR*=9.6 cm/s. Thus, in contrast to [11], in this case, the surface recombination and recombination rates in the SCR are comparable. However, in the case of four recombination mechanisms, when recombination in the SCR is absent, it is necessary to take into account the change in the surface recombination rate to reconcile the theoretical dependences with the experimental ones. This consideration gives a new surface recombination rate, with its 26.6 cm/s minimum value. From the comparison of the total surface recombination rate and recombination rate in the SCR and the new surface recombination rate, it is seen that at the point of maximum power, they are the same. This explains the coincidence of theoretical dependencies in the case of six and four mechanisms.

**Conclusions**

In summary, as shown experimentally in [11] and explained in this paper, a sufficiently high efficiency exceeding 24% can be obtained even when the surface recombination rate is sufficiently high. This is due to the high-quality texturing, which results in a short-circuit current density of the order of 42 mA/cm2.

As our characterization showed, a peculiar feature of SC [11] is also that the exponential index *r* in expression (1) for the surface recombination rate on the excess concentration is 0.62, which is less than unity - the value that usually occurs. We explain this by the fact that in this case the donor charge in the isotype contact is much smaller than the acceptor charge in the anisotype contact.

It was also shown when for the theoretical modeling of the light *J-V* characteristics, dark *J-V* characteristics, short-circuit current, and output power, may be used the approximation of four recombination mechanisms. This can be done when the surface recombination rate significantly exceeds both the recombination rate in the SCR and the rate of non-radiative exciton recombination.

The corresponding criteria that allow using the approximation of the four recombination mechanisms for modeling SCs are satisfied, in particular, for SCs in experimental works [11,17]. At the same time, when calculating the effective lifetime, it is always necessary to take into account recombination in the SCR, otherwise there is no region of decreasing  with decreasing Δ*n* in the region of small Δ*n*.

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**Особливості характеризації та оптимізації високоефективних кремнієвих сонячних елементів при домінуванні поверхневої рекомбінації**

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**Анотація**. В роботі встановлено особливості моделювання процесів фотоперетворення у високоефективних сонячних елементах (СЕ) на основі монокристалічного кремнію для випадку, коли внесок поверхневої рекомбінації значно переважає внески рекомбінації в області просторового заряду (ОПЗ) та безвипромінювальної екситонної рекомбінації за участю домішкових центрів. Показано, що в цьому випадку ключові характеристики процесу фотоперетворення, а саме темнова і світлова вольт-амперні характеристики та залежності вихідної потужності СЕ, отримані з урахуванням та без урахування рекомбінації в ОПЗ та безвипромінювальної екситонної рекомбінації за участю домішкових центрів, практично збігаються між собою.

Результати моделювання порівнювалися з експериментом для СЕ з двох робіт, в яких мали місце зазначені вище умови. Аналіз підтвердив узгодженість теоретичних залежностей, отриманих з урахуванням та без урахування рекомбінації в ОПЗ та безвипромінювальної екситонної рекомбінації, з експериментом. Показано, що оптимізація рівня легування бази та товщини розглянутого сонячного елемента дозволяє збільшити його ефективність з 24,37% до 24,62%.

Результати, отримані в роботі, дозволяють пояснити, чому раніше рекомбінація в ОПЗ не враховувалася при теоретичному моделюванні характеристик СЕ на основі монокристалічного кремнію в переважній кількості робіт, а також показати, що загальний підхід справедливий у випадку будь-якого співвідношення між компонентами струмів рекомбінації в монокристалічному кремнії.

**Ключові слова:** моделювання, кремнієвий сонячний елемент, швидкість поверхневої рекомбінації, рекомбінація в ОПЗ, ефективність фотоперетворення.