Supplementary Information for the paper “**A comprehensive approach to optimization of silicon-based solar cells“**

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**S1. Anderson model**

If we consider a non-ideal heterojunction, we will have to consider the parameters inherent only to this particular structure and the parameters of its manufacture.

Let in the heterojunction under consideration in the near-contact layer of each material. A change in the potential energy of the electron is denoted φ1.2. Then, the equilibrium diffusion potential equals the sum of φ1 and φ2. The changes in the potential energy of the electron are equal to the difference in the thermodynamic work functions.

The electrostatic potential changes continuously, and the field of the pn-junction has one direction. As a result, the vacuum level *E0* on the band diagram changes by an amount equal to φ0.

Charge carriers with high energy can pass through a heterojunction, changing their energy value to φ 0. But for electrons and holes with thermal energies, breaks in energy bands are potential jumps. Consequently, a heterojunction has effective potential barriers with different heights for different charge carriers.

If we consider a nonideal heterojunction, we can propose the existence of a double electrical layer in the near-contact region, a dipole F. The dipole changes the energy band gaps by the value F.

, (1)

where χ1/2 is the thermodynamic work function.

When calculating a specific heterojunction, the first step is calculating the diffusion potential φ0. To do this, you need to know the position of the Fermi level ( *Ec*) on the energy diagram of the structure for each of the heterojunction materials, which depends on temperature (T), the concentration ofthe majority charge carriers, and the density of states in the valence band ( *Nv)* and conduction band (*Nc*). Densities of states can be calculated regarding the effective masses of holes (*mdp*) and electrons (*mdn*).

, (2)

, (3)

where *h* is Planck’s constant, *k* is Boltzmann’s constant, is the longitudinal or transverse component of the effective mass, and *M* is the number of equivalent ellipsoids.

The chemical potential (µ) and diffusion potential (φ 0 ) can then be calculated:

, , (4)

, (5)

where χ 01 and χ 02 are the electron affinity.

Under equilibrium conditions, when integrating the Poisson equation, we obtain the equation for the space charge density (ρ):

, (6)

, (7)

where *N* D is the concentration of donor impurity ions, and *N*a is the concentration of acceptor impurity ions.

Each component of the space charge (the charge of holes, electrons, and impurity ions) can depend on the coordinate for various reasons: inhomogeneous doping, the degree of ionization of the impurity, the concentration of electrons and holes, and potential. Therefore, an exact analytical solution to equation (6) is impossible.

However, we can obtain an analytical solution using the Schottky approximation. The Schottky approximation assumes:

a) impurities are completely ionized; ion concentrations do not depend on potential and follow the law of impurity distribution;

b) each of the conductors has a fairly pronounced impurity character of conductivity;

c) the contact field creates a depletion layer in each of the semiconductors;

e) the thickness of the depletion layers is much greater than the Debye length *l D* for the corresponding semiconductor at the outer boundary of the depletion layer.

Based on the Schottky approximation, in equation (7), we can represent the impurity charge that predominates in a given semiconductor. Then we rewrite (7) in the form:

. (8)

The boundary of the near-contact layer with the electrically neutral volume of the semiconductor is blurred, but due to assumption e), we assume that the layer boundary is sharp. That is, on one side of this boundary, the charge equals (8); on the other, it is zero. The layer depleted of major current carriers due to screening the electric field is called the Schottky layer.

Let us calculate the potential for the case of an anisotype heterojunction with uniform doping of impurities in the Schottky layer approximation. Let us denote *n 1* and *n 2* as the concentrations of the majority charge carriers in the semiconductors that form the heterojunction. The *x-axis path will be directed normally* to the contact plane from the first semiconductor to the second. Let us assume that the coordinate *x* =0 is the contact plane. Let us describe a heterojunction as a double layer of charges:

, ,

, .

The problem reduces to integrating equation (6) with a constant right-hand side. The boundary conditions of the problem are:

, (9)

, (10)

, (11)

, (12)

where σ is the charge density at the interface.

Let us consider a specific type of solution to the Poisson equation when the first semiconductor is of the hole type and the second is of the electronic conductivity type. Let's take φ( *x ≥ x 2* ) = 0. Then we have:

At :

, (13)

. (14)

At :

, (15)

. (16)

Because the conductor's doping condition is uniform, the field strength's dependence on the coordinate is linear, and the potential's dependence is parabolic.

Let us calculate the partial diffusion potential ( ).

; (17)

, *i* =1, 2; (18)

where *Q i* is the charge of the Schottky layers per unit area of the transition. The formula expresses the electric field strength at the interface:

, *i* = 1, 2. (19)

If φ 1 + φ 2 = 1, then from (17) and (18), it follows that ( *Q 1 – Q 2* ) is the canonical equation of the ellipse. Then the semi-axes of the ellipse ( *Q 0i* ) are equal:

. (20)

Let's write the electroneutrality equation

*Q 1 + Q 2 + =0.* (21)

Then, from the system of equations (17), (18), and (21), the solution for the charges of the Schottky layers follows:

(22)

(23)

*.* (24)

From formulas (22) and (23), we can calculate the charges of the Schottky layers. From formula (17), the diffusion partial potentials are calculated, and then, using formulas (18) and (19), the thickness of the Schottky layers can be calculated. The formula expresses layer thickness Schottky (xi)

(25)

**S2. Optimization algorithm**

Optimization of device performance was carried out step by step in the order indicated in Table 1 (descending order R):

* optimization of the p-type doping level of the a-Si:H emitter layer;
* optimization of the thickness of the front layer of the built-in a-Si:H layer of intrinsic conductivity;
* optimization of the thickness of the c-Si single-crystal substrate with n-type conductivity;
* optimization of the thickness of the amorphous layer of a-Si:H p-type conductivity;
* optimization of the degree of doping of a single-crystal c-Si substrate with n-type conductivity;
* optimization of the degree of doping of the rear amorphous layer of a-Si: H n + - conductivity type;
* optimization of the thickness of the rear amorphous layer of a-Si: H n + - conductivity type;
* optimization of the thickness of the back layer of the built-in a-Si:H layer of intrinsic conductivity.

For optimization, the same range of parameter values was used as in the main part, with one additional optimization step - fine-tuning- calculations at additional points located close to the region of maximum efficiency.

The HIT structure's photocell was modeled using the AFORS-HET software package. The software package is designed to model heterojunction solar cells based on crystalline and amorphous silicon and includes a database of parameters for these materials. The detailed operating principle of the AFORS-HET software package is described in [S1]. The simulated solar cells used material parameters from the database integrated into the software, which were measured separately on manufactured samples. The parameters of the monocrystalline and amorphous silicon layers used in the modeling are given in Tables S2.1 and S2.2.

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| **Table S2.1** Parameters of the single-crystal *n* -Si model used in the AFORS-HET software package. | | | |
| Parameter name | Meaning | Parameter name | Meaning |
| The dielectric constant | 11.9 | Density | 2.328 g cm -3 |
| Electron affinity | 4.05 eV | Donor concentration | 2.15×10 17 cm -3 |
| Effective density of states in the conduction band  Effective density of states in the valence band | 2.846×10 19 cm - *3*  2.685×10 19 cm -3 | Acceptor concentration | 0 cm -3 |
| Band gap *E g* | 1.124 eV | Electron/hole surface recombination rate | 10 7 cm/s |
| Effective electron mobility | 1111 cm 2 /V s | Effective hole mobility | 421.6 cm 2 /V s |
| Auger coefficient of electron recombination | 2.2×10 32 cm 6 /s | Auger hole recombination coefficient | 9.9×10 33 cm 6 /s |

|  |  |  |  |
| --- | --- | --- | --- |
| **Table S2.2** Parameters of the amorphous *p* / *n* -Si model used in the AFORS-HET software package. | | | |
| Parameter name | Meaning | Parameter name | Meaning |
| The dielectric constant | 11.9 | Auger coefficient of electron recombination | 20 cm 2 /V s |
| Electron affinity | 3.9 eV | Auger hole recombination coefficient | 5 cm 2 /V s |
| Effective density of states | 10 20 cm -3 | Donor concentration | 10 20 cm -3 |
| Band gap *E g* | 1.72 eV |  | |

Structure optimization data is shown in Figures S3.1 – S3.7 and discussed in section S3. The study determined the optimal parameters of the photocell model of the HIT structure, which are given in Table S2.3.

**Table S2.3** Main parameters of the optimized structure.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | Layer name | | | | |
| Layer options | pa-Si | ia-Si | nc-Si | ia-Si | n + -a-Si |
| Thickness, microns | 0.001 | 0.001 | 200 | 0.003 | 0.005 |
| Alloy level, cm -3 | 0.7×10 20 -1.0×10 20 | - | 1.7∙10 17 | - | 10 20 |
| Final output characteristics:  V OC = 734 mV, J SC = 33.6 mA/cm 2 , FF = 85.06%, efficiency = 20.98% | | | | | |

The presented HIT cell optimization approach based on the top-down sequence shown in Table 3.1 was compared with optimization using inverse ascending and random order of optimization steps. As a result, it was found that the optimization steps algorithm, in which the optimization steps were performed in descending order of the parameter R, led to higher efficiency (20.98%) compared to the results (20.78%) for the increasing sequence and (20.49% ) for a random order of optimization steps. Although the difference in the efficiency of the simulated devices is insignificant, the output parameters of the solar cells, in particular, the thickness of the plate and the level of alloying of the plate, as well as the performance characteristics, are significantly different. When performing optimization in R values in descending order, it was found that the optimal value of the plate thickness is 200 μm. This is very different from the thickness value of 110 µm obtained for the ascending order of optimization steps and 40 µm for the random order of optimization steps. The difference in optimized solar cell performance obtained by different optimization algorithms may be more different in structures that use different values of charge carrier lifetime, surface recombination rate, or recombination and Auger recombination coefficients.

Optimization algorithm p-a-Si:H/i-a-Si:H / n-a-Si:H/i-a-Si:H/n+a-Si:H Cell (ascending order):

* optimization of the thickness of the back layer of the built-in a-Si:H layer of intrinsic conductivity (the result is similar to the decreasing order);
* optimization of the thickness of the rear amorphous layer of a-Si:H-n + - conductivity type;
* optimization of the degree of doping of the rear amorphous layer of a-Si:H-n+ - conductivity type;
* optimization of the degree of doping of a single-crystal c-Si substrate of n-type conductivity;
* optimization of the thickness of the amorphous layer of a-Si:H p-type conductivity;
* optimization of the thickness of a single-crystal c-Si substrate of n-type conductivity;
* optimization of the thickness of the front layer of the built-in a-Si:H layer of intrinsic conductivity;
* optimization of the p-type doping level of the a-Si:H emitter layer.

The results of optimization in reverse order are presented in Table 2 in the main part.

Optimization algorithm p-a-Si:H/i-a-Si:H/n-a-Si:H/i-a-Si:H / n+a-Si:H Cell (random order):

* optimization of the degree of doping of the rear amorphous layer of a-Si:Hn+ - conductivity type;
* optimization of the thickness of a single-crystal c-Si substrate of n-type conductivity;
* optimization of the thickness of the amorphous layer of a-Si:H p-type conductivity;
* optimization of the degree of doping of a single-crystal c-Si substrate with n-type conductivity;
* optimization of the thickness of the front layer of the built-in a-Si:H layer of intrinsic conductivity;
* optimization of the p-type doping level of the a-Si:H emitter layer;
* optimization of the thickness of the back layer of the built-in a-Si:H layer of intrinsic conductivity.

Table 2 presents the results of the main part of optimizing the computer model using random order.

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| Рисунок 81  a) | Рисунок 80  b) |
| Рисунок 79  c) | Рисунок 78  d) |

**Figure S2.1** Optimization data p-a-Si:H/i-a-Si:H/n-a-Si:H/i-a-Si:H/n+a-Si:H PV cells depending on the degree of doping of the p-type emitter. (a) Dependence of the short-circuit current density on the degree of emitter doping, (b) dependence of U xx on the degree of emitter doping, (c) dependence of the fill factor on the degree of emitter doping, (d) dependence of the PV efficiency on the degree of emitter doping.

As the concentration of majority charge carriers in the emitter layer increases, the short-circuit current, fill factor, and efficiency of the photocell increase, as shown in Figure S2.1. The fill factor and efficiency values increase at a charge carrier concentration of 1.5·10 20 cm-3 (Figure S2.1c,d).

The increase in the short-circuit current curve (Figure S2.1a) is due to increased photocurrent generation. It occurs by separating electron-hole pairs by the internal electric field of the pn-junction. This field is comparable to the curvature of energy bands, and the electric field strength depends on the degree of doping of the semiconductors forming the pn-junction.

The open-circuit voltage curve depends on the processes of charge carrier recombination in the structure. Since almost 100% of the solar cell structure is single-crystalline silicon, the open-circuit voltage depends on the processes of charge carrier recombination in crystalline silicon. As a result, the open-circuit voltage curve does not change its dependence on changes in the doping degree of the emitter layer (Figure S2.1b).

The form factor curve (Figure S2.1c) depends on the series and parallel resistance of the structure. Thus, the form factor is influenced by energy barriers and transitions in the band diagram of the structure, the form of which, in turn, depends on the doping level of the layer under consideration. Starting from a concentration value of 1.5·1020 cm-3, the form factor curve begins to increase, which leads to an increase in the efficiency of the photocell (Figure S2.1d).

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| Рисунок 77  a) | Рисунок 76  b) |
| Рисунок 75  c) | Рисунок 74  d) |

**Figure S2.2** Optimization data p-a-Si:H/i-a-Si:H/n-a-Si:H/i-a-Si:H/n+a-Si:H PV cells depending on the thickness of the front built-in i-layer. (а) Dependence of the short-circuit current density on the thickness of the front built-in i-layer, b) dependence of U xx on the thickness of the front built-in i-layer, c) dependence of the fill factor on the thickness of the front built-in i-layer, d) dependence of the PV efficiency on the thickness of the front built-in i-layer layer.

An increase in the thickness of the built-in intrinsic conductivity layer does not lead to a change in the open circuit voltage (Figure S2.2b). Since the built-in layer of intrinsic conductivity leads to better passivation of the surface states of the crystalline substrate, the recombination of charge carriers is reduced. However, due to the amorphous silicon material's quality, the structure's resistance increases, which leads to a decrease in the fill factor (Figure S2.2c) and a drop in the short circuit current (Figure S2.2a). The overall influence of the above-described dependencies negatively affects the efficiency of the photocell. Starting from a built-in layer thickness of 1.3 nm, the efficiency of a photocell of the HIT structure decreases with increasing thickness of the front amorphous built-in layer. However, the point corresponding to a layer thickness of 1.3 nm is the point of maximum efficiency (Figure S2.2d).

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| --- | --- |
| Рисунок 73  a) | Рисунок 72  b) |
| Рисунок 71  c) | Рисунок 70  d) |

**Figure S2.3** Optimization data for p-a-Si:H/i-a-Si:H/n-a-Si:H/i-a-Si:H/n+-a-Si:H PV cells depending on the thickness of the single-crystalline substrate. (а) Дependence of the short-circuit current density I short circuit on the thickness of the single-crystalline substrate, b) dependence of U xx on the thickness of the single-crystalline substrate, c) dependence of the fill factor on the thickness of the single-crystalline substrate, d) dependence of the PV efficiency on the thickness of the single-crystalline substrate

Optimization data for a photocell depending on the increase in the thickness of the silicon crystalline substrate is presented in Figure S2.3. The increase in the efficiency value, as well as the short circuit current, is mainly because it is in the layer of crystalline silicon that photons are absorbed and electron-hole pairs are formed in the pn junction region (Figure S2.3a,d). In the range corresponding to the thickness of crystalline silicon equal to 100 - 200 μm, the efficiency and short-circuit current curves reach saturation. The drop in open-circuit voltage with increasing substrate thickness is because with the thickness of the material, the number of defects deep in the material, which serve as recombination centers for charge carriers, increases (Figure S2.3b).

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| --- | --- |
| Рисунок 69  a) | Рисунок 68  b) |
| Рисунок 67  c) | Рисунок 66  d) |

**Figure S2.4** Optimization data p-a-Si:H/i-a-Si:H/n-a-Si:H/a-Si:H/n+a-Si:H PV cells depending on the thickness of the emitter layer. (a) Дependence of the short-circuit current density I short circuit on the thickness of the emitter layer, b) dependence of Uxx on the thickness of the emitter layer, c) dependence of the fill factor on the thickness of the emitter layer, d) dependence of the PV efficiency on the thickness of the emitter layer

The dependence of the electrical characteristics of the solar cell on the thickness of the amorphous silicon layer of p-type conductivity is shown in Figure S2.4. The photocell's efficiency and other electrical characteristics shown in the figure decrease with increasing layer thickness. The drop in performance is associated with an increase in the series resistance of the structure. The open circuit voltage depends on the light current and saturation current. Since the saturation current is related to the resistance of the structure and the recombination of charge carriers, the open-circuit voltage curve (Figure S2.4b) has a dependence similar to the dependence of the short-circuit current curve (Figure S2.4a). And since the efficiency of the photocell depends on the short circuit current and open circuit voltage, the efficiency value decreases with increasing thickness of the amorphous silicon layer of p-type conductivity (Figure S2.4d).

|  |  |
| --- | --- |
| Рисунок 1  a) | Рисунок 10  b) |
| Рисунок 11  c) | Рисунок 12  d) |

**Figure S2.5** Optimization data p-a-Si:H/i-a-Si:H/n-a-Si:H/i-a-Si:H/n+a-Si:H PV cells depending on the degree of doping of the crystalline substrate n – conductivity type. (а) Дependence of the short-circuit current density on the degree of doping of the crystalline substrate n – n-conductivity type, b) dependence of the open circuit voltageon the degree of doping of the crystalline substrate n-type of conductivity, c) dependence of the fill factor of the degree of doping of the crystalline substrate n-type of conductivity, d) dependence of the efficiency of the solar cell on the degree of doping of the crystalline substrate n-type of conductivity.

An increase in the concentration of the majority charge carriers in the crystalline silicon substrate is accompanied by an increase in the efficiency of the photocell (Figure S2.5). This dependence is associated with an increase in the conductivity of the structure. A change in the degree of doping entails a change in the curvature of the energy bands in the band diagram; such a change affects the short-circuit current and open-circuit voltage (Figure S2.5a,b). An increase in the values of these characteristics is observed in the range from 0 to 10 17 cm -3. However, at a value of about 1017 cm-3, there is an extremum point, and then there is a drop in the efficiency of the solar cell (Figure S2.5d). This behavior of the curve is because as the concentration of the majority charge carriers increases, the probability of Auger recombination in the semiconductor also increases, which entails a decrease in the short-circuit current and open-circuit voltage (Figure S2.5a,b) [S2]. As a result, at the extremum point, the influence of Auger recombination has a more substantial effect on the dependence of the efficiency of the photocell, which leads to a decrease in efficiency.

|  |  |
| --- | --- |
| Рисунок 61  a) | Рисунок 60  b) |
| Рисунок 59  c) | Рисунок 58  d) |

**Figure S2.6** Optimization data p-a-Si:H/i-a-Si:H/n-a-Si:H/i-a-Si:H/n+a-Si:H PV cells depending on the degree of doping of the blocking BSF layer. (а) Dependence of the short-circuit current density on the degree of doping of the blocking BSF layer, (b) dependence of the open-circuit voltageon the degree of doping of the blocking BSF layer, (c) dependence of the fill factor on the doping concentration of the blocking BSF layer, (d) dependence of the efficiency of the solar cell on the degree of doping of the BSF layer.

With an increase in the degree of doping in the BSF layer, the values of the form factor, open circuit voltage, and efficiency increase (Figure S2.6). The concentration of charge carriers in the layer affects the formation of the bending of energy bands at the heterojunction boundary. As soon as the optimal possibility of passing through the energy barrier is created for electrons, and an insurmountable energy barrier is formed for holes, the dependence curves on the graphs stop growing. On the open-circuit voltage, form factor, and short-circuit current graph at the point corresponding to the electron concentration value of 7·1019 cm-3, the curves stop growing, indicating that optimal band straightening has been achieved, as shown in Figure 7. As a result, the PV efficiency graph (Figure S2.6d) enters saturation mode.

Variation of the thickness of the rear i-type aSi:H layer and thickness of the n+-type aSi:H rear layer in the range between 1 and 50 nm (and further) did not result in any change in the device output characteristics. Changing the thickness of the back layer of a-Si:Hn+ − conductivity type in the range from 1 to 50 nm (and further) did not change the device's output characteristics. It should be taken into account that the thickness of the BSF layer should be such that it prevents holes from tunneling through the created energy barrier.

**S3. Modeling Data**

**Table S3.1** Constants used in heterojunction calculations.

|  |  |
| --- | --- |
| Name or designation of the constant | Meaning |
| q, Cl | 1.60 10-19 |
| electron mass in vacuum, kg | 9.10 10-31 |
| Boltzmann constant, eV/K | 8.60 10-5 |
| Pi | 3.14 |
| dielectric constant | 8.85 10-12 |
| Planck's constant, J\*s | 6.63 10-34 |
| Boltzmann constant, J/K | 1.38 10-23 |
| temperature, K | 300 |
| - q, Cl | -1.60 10-19 |
| kT | 4.14 10-21 |

**Table S3.2** Parameters of heterojunction materials at a temperature of 300 K.

|  |  |  |
| --- | --- | --- |
| Parameter | c-Si n-type | a-Si p-type |
| 1 | 2 | 3 |
| m||/m0 | 0.537 | 0.537 |
| m|/m0 | 0.153 | 0.153 |
| M | 6 | 6 |
| md/m0​ | 0.59 | 0.59 |
| ∆E, eV | 1.12 | 1.6 |
| X0, eV | 4.01 | 3.9 |
| 1 | 2 | 3 |
| *E*, eV | 12 | 11.9 |
| mc/m0 | 0.41 | 0.41 |
| Un, cm2/Vs | elec. 1350  holes. 480 | elec. 20  holes. 5 |
| Dn, cm2/s | elec. 34.9  holes. 12.42 | elec. 34.9  holes. 12.42 |
| , With | elec. 2 10 -5  holes. 1 10 -5 | elec. 1.5 10 -13  holes. 1.6 10 -15 |
| E, eV | 4.6 | 4.6 |

**S4. Experimental**

Doped amorphous silicon is a non-photoactive material, which means that in a HIT solar cell, the front p-layer is, in fact, a light filter that reduces the intensity of light passing into the silicon wafer. To increase the photocurrent, a p-layer with a minimum thickness is necessary to ensure the formation of a semiconductor junction. However, it should be noted that the optimal thickness of the amorphous film can be influenced by both technological process limitations and other physical phenomena associated with the heterojunction region or passivation of the surface of a single-crystal silicon substrate.

A study of the effect of reducing the p-layer thickness on a photovoltaic cell was carried out on laboratory elements measuring 100x100 mm. A series of 5 samples was made for each doping level. To prepare the samples, we used commercial Nexolon plates of n-type conductivity with a thickness of 200 μm. The details of samples manufacturing are presented in our earlier work [S3].

The most pronounced effect of reducing the thickness of the p-layer is an increase in the short-circuit current of the cell due to a decrease in light absorption in the short-wave region of the spectrum (Ref. [S3] and Figure 3). The increase in current continues up to a thickness of the p-layer of 8 nm. At smaller thicknesses of the p-layer, the current value begins to decrease, which is apparently due to the degradation of the pn-junction due to a decrease in the thickness of the p-layer to a value less than the thickness of the space charge region. This may also be due to insufficient passivation of surface states on the crystalline silicon substrate. In addition to increasing the short-circuit current, reducing the thickness of the p-layer leads to a slight decrease in the open-circuit voltage and form factor. The decrease in the open circuit voltage is associated with the recombination of charge carriers in the structure. Based on this, as the amorphous silicon layer's thickness decreases, the charge carriers' recombination increases. The combined influence of all these factors leads to the fact that, depending on the PV efficiency on the p-layer thickness, a maximum is observed at a p - p-layer thickness of 10 nm [S3].

**4.2. Optimization of BSF layer thickness**

Unlike the front p-layer, which acts as a light filter, the n-layer is located on the back surface of the solar cell, so its thickness has no significant effect on the parameters of solar cells. At the same time, it is evident that, on the one hand, the n-layer must have a thickness sufficient to form a semiconductor junction, and, on the other hand, reducing production costs requires using an n-layer with a minimum thickness.

The effect of the thickness of the n-a-Si:H layer on the parameters of the HIT PV cell is given in Table S4.1, which collects averaged values for seven samples. As can be seen, the optimal thickness of the n-a-Si:H layer = 20 nm. In the samples under study, the thickness of the front and rear layers of intrinsic conductivity was 7 nm. A series of samples with different thicknesses of the n-layer were also made on wafers of crystalline substrates from another manufacturer.

**Table S4.1** Average values of parameters of HIT PV cells manufactured using wafers of batch 1 and batch 2 n-conductivity type with a thickness of 200 μm, depending on the thickness of the a-Si:H n-layer.

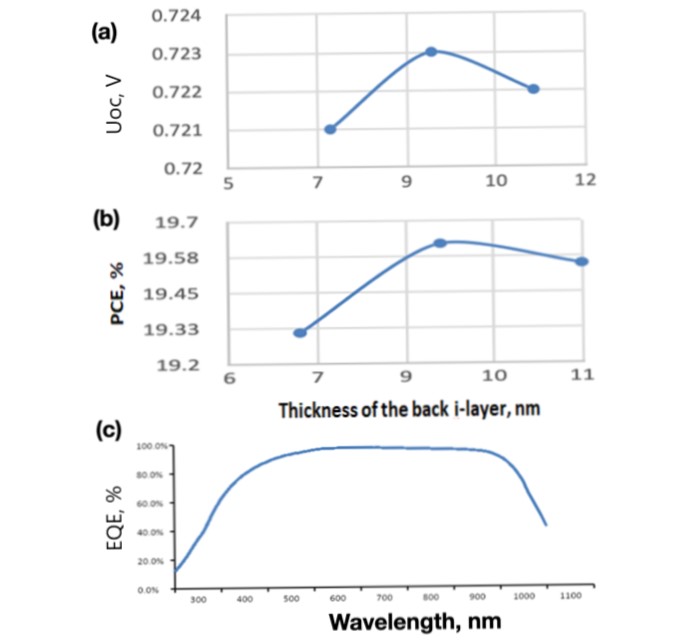
|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Thickness  n-layer | Plate type | ρ  (Ω cm) | VOC  (V) | ISC\_corr  (A) | FF  (%) | Eff. Abs.  (%) |
| 25 nm | 1 | 2.08 | 0.711 | 3.411 | 73.83 | 18.64 |
| 20 nm | 1 | 2.04 | 0.713 | 3.465 | 74.37 | 19.14 |
| 15 nm | 1 | 2.13 | 0.706 | 3.467 | 74.17 | 18.99 |
| 10 nm | 1 | 2.07 | 0.703 | 3.48 | 73.71 | 18.77 |
|  | | | | | | |
| 20 nm | 2 | 2.33 | 0.719 | 3.416 | 73.95 | 18.91 |
| 30 nm | 2 | 2.35 | 0.720 | 3.403 | 74.36 | 18.97 |
| 40 nm | 2 | 2.43 | 0.718 | 3.430 | 73.91 | 18.94 |

As Table S4.1 shows, when using type 2 wafers, a 30 nm thick n-layer results in a higher fill factor value than a 20 nm thick n-layer. Thus, the optimal n-layer thickness may differ for different wafers, which is consistent with computer model studies. This dependence may be because the generation and separation of electron-hole pairs in the device occur in another region of the photovoltaic cell. The blocking layer of n-type conductivity creates a barrier of minority charge carriers.

**4.3. Optimization of the thickness of the built-in i-layer of its intrinsic conductivity type**

The amorphous hydrogenated intrinsic conductivity layer (i-a-Si: H) in the HIT structure, embedded between the crystalline silicon and emitter layer, as well as the blocking layer, plays an essential role in increasing the efficiency of solar cells. The main task of the built-in layer is the passivation of surface states on the crystalline substrate, which makes it possible to increase the lifetime of minority charge carriers to 1500 - 3000 microseconds. To determine the influence of the thickness of the native amorphous silicon layer and the resistivity of the plates on the parameters of the HIT PV, n-type silicon wafers with a thickness of 200 μm were used. The resistivity of the plates varied from 1.3 to 1.4 Ohm cm. The thickness of the ia-Si:H layer varied on both the front and back sides. The thickness of the front layer varied from 5 to 7 nm, while the thickness of the rear layer remained constant (7 nm). Since the absorption of light by a layer of amorphous silicon is critical only from the front side, and the thickness of the ia-Si:H layer determines the value of the open circuit voltage V OC, it was decided to vary the thickness (from 7 to 11 nm, with a constant thickness of the front layer of 7 nm) ia- Si:H layer from the back side, that is, from the n-layer side. As can be seen from Figure S2.4, the optimal value for the thickness of the frontal i-a-Si:H layer is 7 nm, since the open circuit voltage has the highest value precisely at the point corresponding to 7 nm, which is consistent with the computer model studies.

Studies have shown that for the back layer of i-a-Si:H, the optimal value is 9 nm (Figure S4.1), consistent with computer model studies. The higher value of the open circuit voltage at the 9 nm point compared to the value at the 7 nm point can be explained by a decrease in the recombination of charge carriers due to an increase in passivation of the surface states of the crystalline substrate by the amorphous silicon film. In the graph segment from 9 to 11 nm, an increase in the series resistance of the structure has a strong influence, and the open-circuit voltage drops (Figure S4.1b). The shape of the open circuit voltage curve is consistent with the photocell's efficiency curve as a function of the thickness of the built-in back layer (Figure S4.1-a).



**Figure S4.1.** The Uoc (a) and efficiency (b) parameters of a photocell of the HIT structure as a function of the thickness of the rear built-in amorphous layer of intrinsic conductivity. Panel (c) shows the external quantum efficiency of the solar cells.

The presence of a maximum point in the dependencies shown in Figure S4.1 can be explained by the fact that when a film of amorphous silicon of intrinsic conductivity is applied to a crystalline silicon substrate, passivation of the surface states of the substrate occurs. Passivation of the surface of the silicon substrate leads to an increase in the lifetime of minority charge carriers in the semiconductor. The thicker the amorphous film layer, the higher the lifetime of minority charge carriers. This dependence leads to an increase in the efficiency of the photocell with increasing thickness of the amorphous layer. However, amorphous silicon is a material with low charge mobility values. This leads to the fact that an increase in the thickness of the amorphous layer leads to an increase in the resistance of the structure, and the efficiency of the element decreases with increasing thickness of the amorphous layer. This efficiency dependence is consistent with the dependence shown in Figure S4.1b, which shows the open circuit voltage curve. The open-circuit voltage mainly depends on the recombination of charge carriers in the PV structure. A smaller number of surface states at the semiconductor interface leads to less recombination of charge carriers, but increasing the thickness of the amorphous layer increases the possibility of charge recombination. On the graph, the maximum point indicates the thickness of the amorphous layer at which both effects from the built-in layer are equivalent. However, with increasing thickness, the decrease in efficiency becomes faster than its increase.

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