JOURNAL OF NANO- AND ELECTRONIC PHYSICS
Vol. **16** No 1, 01030(5pp) (2024)

ЖУРНАЛ НАНО- ТА ЕЛЕКТРОННОЇ ФІЗИКИ
Том **16** № 1, 01030(5cc) (2024)

OPEN ACCESS

REGULAR ARTICLE

Physics of High Efficiency Silicon Solar Cell with Nanoinclusions of Lead Chalcogenides

M.A. Askarov[1,*], E.Z. Imamov[2], Kh.N. Karimov[2]

[1] *Karakalpak State University named after Berdakh, 230112 Nukus, Uzbekistan*
[2] *Tashkent University of Information Technologies named after Muhammad al-Khwarizmi, 100084 Tashkent, Uzbekistan*

(Received 02 December 2023; revised manuscript received 21 February 2024; published online 28 February 2024)

The question of using non-crystalline silicon as a substrate for an efficient solar cell with many nano heterojunctions based on lead chalcogenide is considered. It is shown that the creation of an efficient solar cell from noncrystalline silicon is also possible at high densities of localized states in the depth of the band gap of silicon. It has been determined that a particularly efficient conversion of solar energy into electricity is possible when heterojunctions of non-crystalline silicon and lead chalcogenides in the nanosized state are combined as components. The manifestation of the effects of multi-exciton generation and multiplication of carriers in lead chalcogenides is taken into account, and the contribution of these manifestations to the process of photocurrent generation is determined.

Keywords: Non-crystalline silicon, Carrier multiplication, Multi-exciton generation, Localized state, Carrier tunneling.

DOI: 10.21272/jnep.16(1).01030 PACS numbers: 73.50.Pz, 73.63.Bd, 84.60.Jt

1. INTRODUCTION

Currently, studies are underway to improve the efficiency of silicon solar cells, when the absorption of each photon is accompanied by the appearance of light electricity. This multifactorial problem is solved taking into account the characteristics of solar radiation, as well as various properties and structures of the solar cells themselves.

Radiation factors are the solar constant equal to 1353 W/m^2 and its maximum value in the territory of Uzbekistan (at latitude 41^o÷43^o) about 900 W/m^2. The constants have different energy distributions, i.e. they have a strong influence on the frequency dependence of the photocurrent. The value of 900 J/(s·m^2) corresponds to the light passing through the dense atmosphere and its energy absorbed by a surface unit per unit time, in clear weather at noon. This also takes into account the value of the atmospheric mass (AM), which determines the spectral characteristic of solar radiation on the earth's surface, corresponding to the relative thickness of the passage of visible light. The minimum daily average annual value of AM corresponding to the local astronomical noon for Uzbekistan corresponds to AM-1.5 (for Belarus AM-2.2; for Germany AM-2.0; for Ukraine AM-1.6; for California AM-1.3 [1]).

As for the properties of materials and structures of solar cells, the paper considers the use of non-crystalline silicon as a substrate for an efficient solar cell. It is proposed to implement this task in combination with the creation of nano heterojunctions (NHJs) from another semiconductor on the substrate surface.

2. STRUCTURE OF SOLAR PANELS

The main component of the technical devices of solar energy is a solar panel (Fig. 1(1)). In turn, the solar panel consists of many solar cells connected in parallel and in series (Fig. 1(2)), on which solar electricity is generated. The main conversion process in solar cells is carried out in a variety of diode or contact structures (*p-n* junctions or hetero junctions).

A solar cell (circled in Fig. 1(1)) consists of many NHJs (Fig. 1(2)), an enlarged schematic model of one of them with an adjacent section of silicon in the form of a parallelepiped (with sides "L" and "b") shown in Fig.1(3). The frontal square profile of the NHJ (Fig. 1(4)) has an area of "a^2", the silicon area adjacent to it is "$b^2 - a^2$". The thickness of the NHJ is "d", and the thickness of its space charge region is "R_0".

The paper proposes a solar cell with many nano heterojunctions on the silicon surface (NHJ <PbX:Si>), in which the second contact material is nanosized lead chalcogenides (PbX, where X can be S, Se, Te).

The formation of a nano heterojunction on the Si surface is a two-stage process:

– by the method of molecular beam epitaxy [2, 3] based on the principle of self-organization of matter [4-8] on the Si surface, the growth of stable pyramidal islands of PbX nanoinclusions begins;

– simultaneously with growth, the nanoinclusion contact with the substrate is formed and NHJ <PbX:Si> is formed.

In a number of early works [3, 8-10], the temperature ranges and illumination intensity ranges, as well as the optimal parameters of lead chalcogenides (shapes, sizes,

---

[*] Correspondence e-mail: asqarovm@list.ru

Cite this article as: M.A. Askarov et al., *J. Nano- Electron. Phys.* 16 No 1, 01030 (2024) https://doi.org/10.21272/jnep.16(1).01030

density, stability) were studied in detail. Experimental studies and their model substantiation made it possible to determine the most favorable conditions for the stable manifestation of quantum phenomena in nano heterojunctions based on PbX (such as multi-exciton generation and the effect of current carrier multiplication).

It is from these results that:

– the possibility of growing stable pyramidal PbX islands with {100} faces coinciding with the orientation of the silicon substrate;

– the possible value of the distribution density of the NHJ on the surface of the substrate (about 10^{11}-10^{12} m^{-2});

– possibilities of lead chalcogenide due to multi-exciton generation and the effect of multiplication of current carriers to effectively convert almost the entire range of the solar radiation spectrum into electricity.

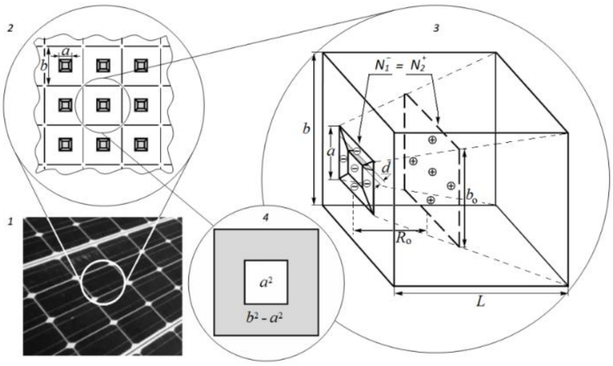

Fig. 1 – The multicomponent structure of solar panels

3. RESULTS AND ITS DISCUSSION

3.1 Features of Non-Crystalline Silicon as a Solar Cell Substrate

Non-crystalline materials retain short-range order at distances comparable to the size of crystallites, that is, on the order of several tens to hundreds of angstroms. The electrical conductivity of such structures (besides the insignificant contribution of free carriers) is determined to a large extent by the tunneling of carriers from the local energy states of Si to the boundary levels of PbX nanoinclusions. The acquisition of electrons of the Si boundary states is carried out by electron hops from one bulk local level in the Si band gap to another [11, 12].

The density of localized states in the band gap (of both donor and acceptor nature) can be $10^{24}\div10^{26}$ m$^{-3}\cdot$eV^{-1}. In this case, the Fermi level – is located, as a rule, closer to the middle of the band gap. Small distances between local discrete states in noncrystalline materials (high density of local states means small distances between defects) create favorable conditions for tunneling and electron hopping through them (even at relatively high temperatures).

Noncrystalline silicon as a substrate is able to form an efficient solar cell in combination with lead chalcogenide nanoinclusions. Many nano heterojunctions can occur in this solar cell, with their characteristic high probability of tunneling processes [13-16].

Schematically, this process of formation of NHJ <PbX:Si> is shown in Fig. 2, in which a hump-shaped curve of "tails" of n-density of states is shown for simplicity only of a donor nature in the Si band gap.

In nanoscale lead halides PbX, the energy levels of electrons and holes are discrete [17, 18].

The formation of a heterojunction between PbX and Si with a single Fermi level is accompanied by electron transitions from Si to PbX nanoinclusions. From the levels a_1, a_2, a_3, …, formed by the "tails" of the density of the local energy states of silicon lying deep in the bandgap (dotted density curve), electrons tunnel to the multi-exciton levels of nanoinclusions c_1, c_2, c_3, … only when these levels coincide (for example, a transition of type $a_1 \rightarrow c_1$).

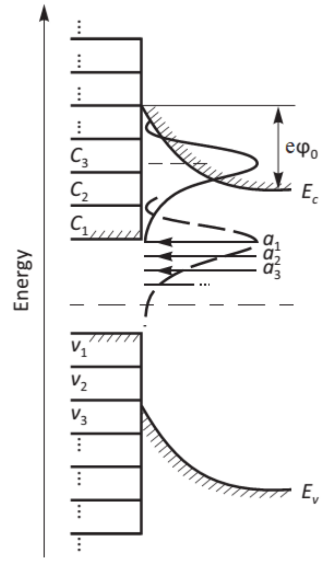

Fig. 2 – The scheme of formation of the nano heterojunction: NHJ <PbX:Si>

This transition is accompanied by the appearance of a φ_i – contact potential and a corresponding shift by $e\varphi_i$ of the hump-shaped curve of silicon localized states upward in energy. Then there is a second transition ($a_2 \rightarrow c_1$), when a_2 coincides with the level c_1. So, until the Fermi energies of both contacting materials (F_{Si} and F_{PbX}) are equalized as a result of tunneling transitions of silicon electrons from deep levels a_i to the multi-exciton state c_1 of the PbX nanoinclusion. In this case, the final value φ_o is established – the contact potential difference of the formed NHJ <PbX:Si>. The total number of electrons transferred from Si to PbX N_1 is determined by C – the electric capacitance of the states in PbX "c_1" and the value φ_0:

$$N_1 = \frac{C \cdot \varphi_0}{e}, \qquad (3.1)$$

where $C = \dfrac{\varepsilon_{PbX} \cdot \varepsilon_0 \cdot a^2}{d}$, $\varepsilon_0 = 8.85 \cdot 10^{-12}$F/m, ε_{PbX} – is the permittivity of PbX.

Such an amount is provided by hopping and tunneling of electrons of local deep energy states in the band gap. Their number N_2 (equal to N_1) is determined by the value:

$$\exp\left(-2r\sqrt{\frac{2m^*(e\varphi_i - E)}{\hbar^2}}\right), \qquad (3.2)$$

i.e., the probability of electron tunneling from the a_i level (at the boundary with the nanoinclusion) to the boundary levels of the PbX nanoinclusions. Here r is the length of tunneling ($a_i \to c_1$) through the barrier with height $\{e\varphi_i - E\}$ of an electron with effective mass m^*.

By varying these three parameters of the electron tunneling probability (r, $\{e\varphi_i - E\}$ and m^*), it is possible to determine their most optimal values, which ensure the equality of the total number of tunneled electrons N_1 and N_2 – the number of electrons transferred to PbX from local deep energy states of the bandgap Si.

Each nanoinclusion can capture electrons only from a certain part of the silicon substrate. This volume, from which the electrons passed into PbX, forms a space charge region (SCR) in Si. Fig.1 (3) shows this area in the form of a rectangular truncated pyramid with bases a^2 and b_0^2, height R_0 (R_0 is the SCR width).

The number of electrons at local levels that are able to tunnel in PbX is determined by the relation

$$N_2 = \xi \cdot b^2 \cdot L \cdot n \cdot \exp\left(-2r\sqrt{\frac{2m^*(e\varphi_i - E)}{\hbar^2}}\right), \qquad (3.3)$$

where $\xi = \frac{1}{3}\gamma\left[\left(\alpha + (1-\alpha)\gamma\right)\cdot\left(2\alpha + (1-\alpha)\gamma\right) + \alpha^2\right]$ determines the fraction of the SCR in relation to the volume "$b^2 \cdot L$", expressed in terms of dimensionless quantities $\alpha = a / b$; $\gamma = R_0 / L$.

As a result of the formation of a single Fermi level (or when $N_1 = N_2$), the nano heterojunction is completely formed. Equalizing expressions (3.1) and (3.3), we get the relation:

$$\frac{\varepsilon_{PbX} \cdot \varepsilon_0 \cdot a^2 \cdot \varphi_0}{e \cdot d} = \xi \cdot b^2 \cdot L \cdot n \cdot \exp\left(-2r\sqrt{\frac{2m^*(e\varphi_i - E)}{\hbar^2}}\right). \qquad (3.4)$$

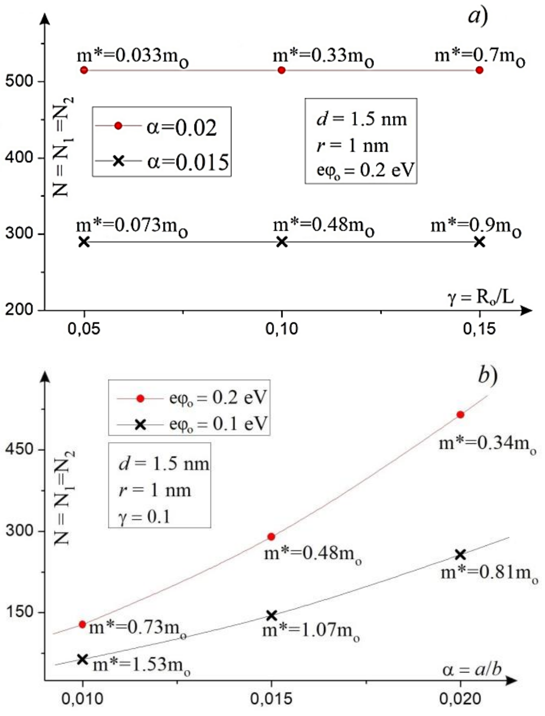

Fig. 3 – Values of effective masses at which $N = N_1 = N_2$

From (3.4), we determine by mathematical modeling the optimal values of the parameters of the PbX nanoinclusion and the Si substrate, at which $N_1 = N_2$.

From the condition of equality of N_1 and N_2 (3.1 and 3.3) for specific values of α (Fig.3(a)), changing γ, and also for specific values of γ (Fig.3(b)), changing α, are determined (for two values of $N_1 = 290$ and $N_1 = 515$) effective mass values ($\gamma = 0.05$; 0.1; 0.15 and $\alpha = 0.01$; 0.015; 0.02).

From Fig. 3(a) it follows that, with a constant value $\alpha = a / b$ (when $e\varphi_o$ = const), the equality $N_1 = N_2$ is achieved for any values of $\gamma = R_0 / L$. As γ increases, the effective electron mass also increases, since an increase in Ro leads to an increase in N_2 and the SCR volume. The growth of N_2 is retarded by a decrease in the tunneling probability (an increase in the effective masses m^*).

From Fig. 3(b) it follows that with a constant value $\gamma = R_0 / L$ and $e\varphi_o$ = const, the equality $N_1 = N_2$ is achieved with an increase in "a^2" – the area of PbS (or the value of N_1), and a corresponding increase in N_2 leads to a decrease in the effective mass m^*.

3.2 The Process of Generating Solar Electricity

The efficiency of the photo conversion process (that is, when the absorption of photons is accompanied by the appearance of light electricity) is determined by the physical properties of the contacted NHJ materials: Si - silicon and lead chalcogenide. Light electricity in nano heterojunctions is largely determined by various quantum effects [15, 16], many of which are especially pronounced in lead chalcogenides (PbX). Being a nano-sized lead chalcogenide, PbX makes a special contribution to the efficiency of the photoconversion process. In particular, we are talking about the quantum effect of multi-exciton generation (MEG) and the effect of current carrier multiplication (CM) [14, 15, 19-21]. These effects determine the process of effective absorption of light by the illuminated surface (Fig. 1(4) area "a^2") at different values of the quantum yield (β) in the corresponding intervals of the solar radiation spectrum.

According to [17, 18], in the range of solar radiation, β takes 4 values for PbS and 7 for PbSe. For example, in Table 1 for PbS, the ranges of manifestation of the effects of carrier multiplication and multi-exciton generation are indicated for various four values of ß.

For NHJ <PbS:Si> N_{PbS} is the number of effectively absorbed photons (that is, the number of generated electron-hole pairs) by the frontal part of the NHJ with area "a^2". It is determined by multiplying the peak intensity of solar radiation in the territory of Uzbekistan (900 W/m^2) by β (range number from 1 to 4) and the share of absorbed solar radiation energy in the corresponding range β. The resulting ratio is divided by the average photon energies in the corresponding β ranges. It is determined by the ratio:

$$N_{PbS} = \sum N^i_{PbS} = a^2 \cdot 5.26 \cdot 10^{21}, \qquad (3.5)$$

that is, summation over all four ranges (i runs from 1 to 4 in PbS). The results of subsequent calculations and their analysis are presented below for PbS (Table 1).

Table 1 – Ranges of the effects of carrier multiplication and multi-exciton generation in nanoclusions PbS

Intervals (eV) in the effective absorption spectrum of PbS with different β- quantum outputs	0.3÷1.2 $\beta \leq 1$	1.2÷1.8 $\beta \leq 2$	1.8÷2.4 $\beta \leq 3$	2.4÷3 $\beta \leq 4$
Share of light absorption energy (%)	16.0	18.0	20.0	18.0
The average value of the radiation energy (eV)	1.05	1.55	2.25	2.55
The number of effectively absorbed photons by the front part of the NHJ in PbS (phot/(s ·m^2) – N^i_{PbS})	$a^2 \cdot 0.86 \cdot 10^{21}$	$a^2 \cdot 1.3 \cdot 10^{21}$	$a^2 \cdot 1.5 \cdot 10^{21}$	$a^2 \cdot 1.6 \cdot 10^{21}$

In the silicon region of NHJ <PbS:Si>, the number of effectively absorbed photons N_{Si} characterizes the spectrum of effective light absorption on the area "$b^2 - a^2$" and is determined by the fraction of absorbed radiation energy in the range of 1.1 ÷ 1.8 eV (excluding impurity absorption):

$$N_{Si} = \left(b^2 - a^2\right) \cdot 1.2 \cdot 10^{21} . \tag{3.6}$$

The average area of the silicon substrate adjacent to the NHJ (b^2) can effectively absorb a maximum of 25 % of solar radiation, that is, when $a^2 << b^2$ (or $a^2/b^2 << 1$) the contribution of this average area will be small. In the case ($a^2/b^2 \leq 1$), when "a", large-dimensional effects may disappear [7]. Therefore, in order to search for the most optimal value of the area of the NHJ, it is only necessary to increase its area "a^2" within reasonable limits.

From the relations (3.5) and (3.6) obtained, the total number of absorbed photons in both parts (N_{PbS} and N_{Si}) is determined:

$$\begin{aligned} N = N(a,b) = N_{PbS} + N_{Si} = \\ = a^2 \cdot 4.06 \cdot 10^{21} \cdot \left[1 + \left(b^2 / a^2\right) \cdot (1{,}2 / 4{,}06)\right] \end{aligned} . \tag{3.7}$$

It can be seen that almost the entire range of incident solar radiation is effectively absorbed in PbS due to successive manifestations of the effect of multi-exciton generation (MEG) and the effect of current carrier multiplication (CM). And although the absorption of solar radiation in PbS is relatively small (about 0.2 %), its contribution to the photocurrent is significant due to the relatively large value of the contact field in NHJ <PbS:Si>.

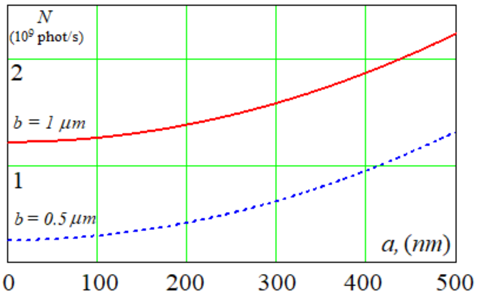

Fig. 4 – Graph of dependence $N = N(a,b)$

And in Si, mainly a limited range of incident solar radiation (1.0÷1.7 eV) is effectively absorbed. However, the electron-hole pairs produced in it are effectively separated in the NHJ contact field.

Fig. 4 shows a graph (3.7) – dependences $N = N(a, b)$. It can be seen from the figure that in the range of real changes "a" from 10÷30 nm, $N = N(a,b)$ practically does not change.

The increase in N with a hypothetical growth of "a" occurs due to an increase in the area of the NHJ (an increase in its electric capacity). It also increases with an increase in the size of the silicon area adjacent to it – "b". However, an excessive increase in "b" is accompanied by an undesirable decrease in the amount of NHJ on the substrate surface, and an increase in "a" can significantly reduce the effective life of the solar panel due to the risk of coagulation of dispersed nano combinations. Therefore, the choice of the optimal values "a" and "b" is determined by the specific operating conditions of the solar panel. In practice, the most acceptable values are: a = 20 nm, b = 1000 nm.

Thus, using the NHJ <PbS:Si> as an example, it is shown that the generation of solar electricity is determined only by the effective absorption of photons, that is, when the absorption of photons is accompanied by a photocurrent. Otherwise, the absorption causes a certain heating of the solar cell, which may degrade its efficiency.

4. CONCLUSIONS

The possibility of using disordered silicon as one of the components of a solar cell is theoretically investigated, assuming an improvement in its efficiency.

The creation of an efficient solar cell in this way turned out to be possible at high densities of localized states in the depth of the band gap of silicon. This occurs when two materials are combined as heterojunction components: disordered silicon and nanosized lead chalcogenide.

Consideration of the effects of multi-exciton generation and multiplication of current carriers in nanosized lead chalcogenides has significantly expanded the effective absorption spectrum of a solar cell with many NHJ <PbS:Si>.

REFERENCES

1. V.F. Gremenok, M.S. Tivanov, V.B. Zalessky, *Solar cells based on semiconductor materials* (Minsk: Publishing House of the BSU Center: 2007).
2. V. Stancu, E. Pentia, A. Goldenblum et al., *Romanian Journal of Information Science and Technology* **10** No 1, 53 (2007).
3. A. Raab, G. Springholz, *Appl. Phys. Lett.* **81** No 13, 2457 (2002).
4. A.I. Gusev, *Nanomaterials, Nanostructures, Nanotechnologies* (M.: FIZMATLIT: 2005)
5. N.N. Ledentsov, V.M. Ustinov, V.A. Shchukin et al., *Semiconductors* **32** No 4, 343 (1998).
6. I.R. Prigozhin, I. Stengers, *Time, Chaos, Quantum. Solving the Paradox of Time* (M.: 2000).

7. H. Haken, *Synergetics* (Springer: Berlin-Heidelberg: 1997).
8. G. Springholz, V. Holy, M. Pinczolits, G. Bauer, *Science* **282**, 734 (1998).
9. S.P. Zimin, E.S. Gorlachev *Nanostructured Chalcogenides of Lead: Monograph*, (Yaroslav State University named after P. G. Demidov: 2011).
10. A. Raab, G. Springholz, *Appl. Phys. Lett.* **77** No 19, 2991 (2000).
11. A.I. Gubanov, *Quantum Electronic Theory of Amorphous and Liquid Semiconductors* (Publishing House of the USSR Academy of Sciences: 1963).
12. N. Mott, E. Davis, *Electronic Processes in Crystalline Substances* (Mir Publishing House: 1974).
13. E.Z. Imamov, R.A. Muminov, R.H. Rakhimov, H.N. Karimov, M.A. Askarov, *Comput. Nanotechnol.* **9** No 4, 70 (2022).
14. M.A. Askarov, E.Z. Imamov, R.A. Muminov, K.A. Ismaylov, *Science and Education in Karakalpakstan* No 4-2, 226 (2022).
15. M.A. Askarov, E.Z. Imamov, R.A. Muminov, *Science and Innovation* **2**, 226 (2023).
16. E.Z. Imamov, Kh.N. Karimov, C.C. Khalilov, A.E. Imamov, *Science and Innovation* No 3, 367 (2022).
17. R.D. Schaller, V.I. Klimov, *Phys. Rev. Lett.* **92**, 186601 (2004).
18. V.I. Klimov, *J. Phys. Chem. B* **110**, 16827 (2006).
19. M. Wolf, R. Brendel, J.H. Werner, H.J. Queisser, *J. Appl. Phys.* **83**, 4213 (1998).
20. R. Ellingson, M.C. Beard, J.C. Johnson, P. Yu, O.I. Micic, A.J. Nozik, A. Shabaev, A.L. Efros, *Nano Lett.* **5**, 865 (2005).
21. B. Sun, A.T. Findikoglu, M. Sykora, D.J. Werder, V.I. Klimov, *Nano Lett.* **9** No 3, 1235 (2009).

Фізика високої ефективності кремнієвого сонячного елемента з нановключеннями халкогенідів свинцю

M.A. Askarov[1], E.Z. Imamov[2], Kh.N. Karimov[2]

[1] *Karakalpak State University named after Berdakh, 230112 Nukus, Uzbekistan*
[2] *Tashkent University of Information Technologies named after Muhammad al-Khwarizmi, 100084 Tashkent, Uzbekistan*

Розглянуто питання використання некристалічного кремнію в якості підкладки для ефективного сонячного елемента з безліччю наногетеропереходів на основі халькогеніду свинцю. Показано, що створення ефективного сонячного елемента з некристалічного кремнію також можливе при високій щільності локалізованих станів у глибині забороненої зони кремнію. Було визначено, що особливо ефективне перетворення сонячної енергії в електричну можливе, коли гетеропереходи некристалічного кремнію та халькогенідів свинцю в нанорозмірному стані поєднуються як компоненти. Враховано прояв ефектів мультиекситонної генерації та розмноження носіїв у халькогенідах свинцю та визначено внесок цих проявів у процес генерації фотоструму.

Ключові слова: Некристалічний кремній, Множення носіїв, Мультиекситонна генерація, Локалізований стан, Тунелювання носіїв.