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REGULAR ARTICLE

Research of Electrophysical Processes in a Silicon Solar Cell with Many Surface Nanoheterojunctions

M.A. Askarov[1,2,*], E.Z. Imamov[3], Kh.N. Karimov[3]

[1] *Karakalpak State University named after Berdakh, 230112 Nukus, Uzbekistan*
[2] *Tashkent Institute of Chemical Technology, 100011 Tashkent, Uzbekistan*
[3] *Tashkent University of Information Technologies named after Muhammad al-Khwarizmi, 100084 Tashkent, Uzbekistan*

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Based on studies of various electrical manifestations and properties of non-crystalline silicon and crystalline lead chalcogenides in the nanoscale state, for the first time it was concluded that it is possible to create a highly efficient solar cell based on them. It has been demonstrated that the phenomena of carrier multiplication and multiexciton generation play a significant role in ensuring high efficiency, due to which a significant reduction in energy losses associated with heating the solar cell is possible. The dependence of the efficiency of a solar cell on the properties of the materials of its components has been determined. The features of the formation of the contact field of a solar cell are shown and its electrical parameters are calculated. The contribution of the absorption of high-frequency photons to the efficiency of the solar cell is calculated.

Keywords: Energy, Photocell, Photocurrent, Nanoheterojunction, Structure, Non-crystalline, Efficiency.

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1. INTRODUCTION

Currently, high efficiency of solar industry is achieved through the use of contact structures (solar cells – SCs) made of expensive monocrystalline silicon in solar panels (or, in extreme cases, the use of poly-crystalline silicon for this). It is known that the solar cell is the main device that converts solar energy into electricity in any solar energy systems.

As for the use of non-crystalline silicon as one of the contact materials of a solar cell and the expectation of high efficiency from its contact field, in practice this was considered absolutely unpromising and even meaningless. This circumstance is due to the fact that in non-crystalline silicon almost all electrons are localized in defective potential wells and are unable to diffuse over long distances. This means that the contact field is not formed, that is, the formation of a solar cell is not possible.

However, in works [1-5] results were obtained:

– asserting an improvement in the transforming properties and efficiency of a solar cell with a single p-n junction while reducing its size [1, 2];

– demonstrating a significant increase in the efficiency of photoconversion in nanocrystals of lead chalcogenides on the surface of amorphous silicon due to the effect of multiexciton generation (MEG) and the phenomenon of current carrier multiplication (CM) [3, 4];

– determining the most likely preferential self-organizing growth of "islands" of the nanocrystal of lead chalcogenides precisely on random crystallites of non-crystalline silicon [5].

Based on these results, in [6-23] the problem of creating SC NHJs – a solar cell with many nanoheterojunctions (per square cm about 10^8-10^{10}) on its surface from non-crystalline silicon was considered.

From these studies it follows that in order to create a fairly highly efficient solar cell based on non-crystalline silicon, it is important to choose nanocrystals of lead chalcogenide, that is, PbX NCs (X can be Sulfur-S, or selenium – Se, or tellurium – Te), as its other component.

In addition, it is clear that solar panels created from parallel and series-connected solar cells with many heterojunctions (<Si:PbX>) are able to provide stable performance and operation for a long time in open areas with harsh climatic conditions (tens of years). In other words, the reality of creating effective <Si:PbX> based on a combination of cheap non-crystalline silicon and nanocrystals of lead chalcogenide is shown. It is with this combination of contacting materials that <Si:PbX> is able to retain its transformative qualities.

2. PROPERTIES OF SOLAR CELL MATERIALS THAT ENSURE ITS EFFICIENCY

Let's consider the properties of materials of a solar cell with many heterojunctions <Si:PbX>, ensuring its efficiency.

* Correspondence e-mail: asqarovm@list.ru

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Features of non-crystalline silicon. The general concepts of band theory, despite the disordered arrangement of atoms, are conditionally applicable to non-crystalline materials. The concepts of permitted and prohibited zones are acceptable to them. The band gap can be determined, as in crystalline semiconductors, by measuring optical phenomena.

Real non-crystalline semiconductors consist of small crystalline inclusions (crystallites) or other irregularities in homogeneity. Crystallite sizes range from one to 10 nm.

In the band gap of a non-crystalline semiconductor, there is a characteristic quasi-continuous spectrum of localized defect energy states (LDES), the appearance of which along the "band gap" of Si is shown in Fig. 1. Each electron in these states is characterized by the defect coordinate r, its binding energy E(r) and with the energy density along the "band gap" (both donor and acceptor nature) g(E) [24]. This density is determined by the concentration of defects $n_0 = 10^{24} \div 10^{26}$ m^{-3} [24, 25]. At such concentration values, the average side of the square b, completely covering one crystallite located at a distance $r = b$ from the neighboring defect, is equal to 2.15 ÷ 21.5 nm (therefore $n_o = r^{-3} = b^{-3}$).

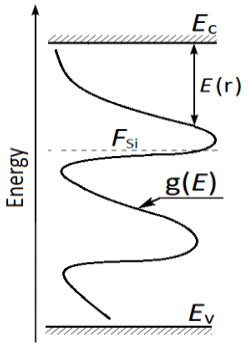


Fig. 1 – View of localized defect energy states in the "band gap" of noncrystalline silicon

Due to the deep location of localized defect energy states in the "band gap", their ionization with the formation of free current carriers is unlikely.

The Fermi level is fixed near the middle of the "band gap". Energy levels near the Fermi energy owe their origin to natural lattice defects such as crystallites

Relatively small distances r - between deep local discrete energy states allow mutual transitions between them [24, 25].

Features of nanocrystalline lead chalcogenide. Nanocrystals of lead chalcogenides grow on random crystallites near the silicon surface in the form of individual "islands" of nanoinclusions [26–31].

Nanocrystals of lead chalcogenide are characterized by:

– an energy spectrum consisting of narrow "quasi-levels" C_i and V_i, similar to discrete states of a single atom (Fig. 2);

– the distances between individual sublevels C_i of free and V_i filled zones are equal to each other due to the practical equality of the corresponding effective masses of current carriers ($m_p \approx m_n$) [32], and the size of this distance is inversely proportional to the size of the nanoinclusion (the smaller the size, the wider the sublevels are located in C_i and V_i);

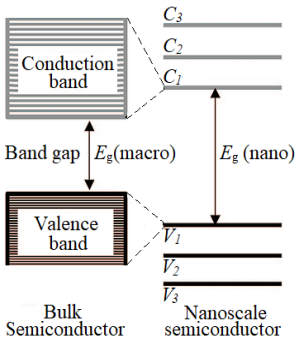


Fig. 2 – Change of energy bands of a semiconductor in nanoscale states

– the width of the "gap band" (E_g^{PbX}) in all PbX increases with a decrease in their dimensions (for exam-ple, E_g^{PbS} at 300 K is 0.39 eV, and in nanosized PbS it increases by 1.3–2 times [32]);

– PbX crystals have very high ε_{PbX} – static dielectric constants, which determines their high electrical capacity (for example, at 77 K: $\varepsilon_{PbX} = 178 \div 184$, $\varepsilon_{PbSe} = 227$, $\varepsilon_{PbTe} = 1300$ [33]);

– in PbX it is possible to exhibit large values of β - quantum yield (for example, in PbS $\beta = 4$, and in PbSe $\beta = 7$), providing an increase in the efficiency of SCs when absorbing high-frequency light due to the manifestation of multiexciton generation of carriers in them [34] and the phenomenon carrier multiplication [35].

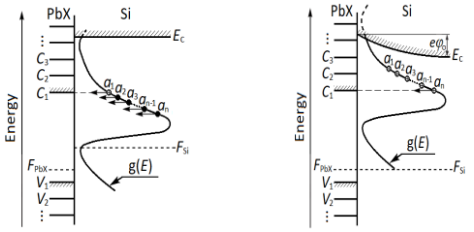
The above features of NCs PbX and non-crystalline silicon justify the possibility of creating efficient solar radiation converters.

3. RESULTS AND DISCUSSIONS

3.1 Mechanism of Formation of the Contact Field in the Nanoheterojunction <Si:PbX>

The mechanism of formation of the contact field usually begins at the moment when the Fermi levels of the contacting materials differ from each other and is carried out by mobile free current carriers. However, in non-crystalline silicon, the mobility of carriers is carried out mainly due to their jumps between neighboring states of the band gap [24]. From these states, an electron can go to PbX, whose static Fermi level is lower than that of silicon by the amount $\Delta\mu = F_{Si} - F_{PbX}$. The transition will occur if their corresponding states coincide. A diagram of the dynamics of such a <Si:PbX> formation process is shown in Fig. 3. It can be seen that PbXs interact with silicon only when the energy levels a_i and C_1 coincide.

The formation of a contact will begin when the level a_1 of the electron in Si is equal to the energy of the first multiexciton level C_1 in PbXs. The transition of the first electron from level a_1 will cause:



a b

Fig. 3 – Dynamics of the formation of <Si:PbX>: at the beginning ($F_{Si} > F_{PbX}$ (a)), and at the end of the process ($F_{Si} = F_{PbX}$ (b))

– transformation of localized defect energy states into a positively charged defect state (conditionally into a "hole"), thereby fixing the beginning of the formation of a space charge region;

– the appearance of a certain proportion of contact potential $\varphi_1 = \varphi_0$/N;

– deformation of the energy spectrum of Si with the appearance of some bending of its "conduction band", equal to the difference in energies of two successive levels $e \cdot \varphi_1 = (a_1 - a_2)$;

– jump-like shift in energy of the density of defect states $g(E)$.

The next transition cycle of the second electron will occur only when the energy of level a_2 coincides with level C_1 (a_2 coincides with C_1 due to a jump in the con-tact field and the corresponding bending of the bands. In this case, the formation of a second hole, an additional contact field ($a_2 - a_3$) and subsequent coincidence of level a_3 with the multiexciton level C_1, conditions appear for the transition of the third electron with the formation of the third "hole".

And so on until comparing the Fermi levels ($F_{Si} = F_{PbX}$) with the transition of N electrons from Si to PbX.

As a result, the nanoheterojunction <Si:PbX> is finally formed with the formation of a space charge region (SCR) along the length R in silicon, and the final value of the contact potential difference $\varphi_0 = \Delta\mu/e$ is established.

3.2 Determination of the Electrical Parameters of the Contact Field of the Nanoheterojunction <Si:PbX>

The electrical parameters of the contact field of the <Si:PbX> nanoheterojunction are determined from the solution of the Poisson equation [25]:

$$\frac{d^2\varphi}{dx^2} = -\frac{\rho}{\varepsilon_{Si}\varepsilon_0} \qquad (1)$$

where ε_{Si} is the dielectric constant, ρ is the space charge density in the contact field, ε_0 is the dielectric constant.

Here ρ – the charge density of ions of localized defect energy states (or "holes") is assumed to be a linear, uniform and homogeneous value.

Integration of the equation is carried out taking into account the boundary conditions of continuity $\varphi(x)$ and $d\varphi/dx$ along the entire field, as well as the presence of a connection between the electric field strength vector $E(r)$ and its potential $\varphi(r)$: $E(r) = -\text{grad}\varphi$.

In the one-dimensional case, the solution has the form:

$$E(x) = \frac{\rho(x-R)}{\varepsilon_{Si}\varepsilon_0} = E_0\left(\frac{x}{R} - 1\right) \qquad (2a)$$

$$\varphi(x) = -\frac{\rho(R-x)^2}{2\varepsilon_{Si}\varepsilon_0} = -\varphi_0\left(1 - \frac{x}{R}\right)^2 \qquad (2b)$$

where $R = \left(\frac{2\varepsilon_{Si}\varepsilon_0 L\varphi_0}{en_0}\right)^{\frac{1}{3}}$, $N = \left(\frac{2\varepsilon_{Si}\varepsilon_0 L\varphi_0}{e}\right)^{\frac{1}{3}}$, L – silicon thickness, n_0 – defect concentration, E_0 and φ_0 – values of E(x) and φ(x) at $x = 0$:

$$E_0 = \left(\frac{4en_0\varphi_0^2}{\varepsilon_{Si}\varepsilon_0 L}\right)^{\frac{1}{3}}, \quad \varphi_0 = \frac{eN^3}{2\varepsilon_{Si}\varepsilon_0 L} \qquad (3)$$

From the obtained relations it is clear that the values of E_0 and R at different values of φ_0 depend differently on no and L:

E_0 increases as $n_0^{1/3}$, and R, on the contrary, decreases as $n_0^{-1/3}$;

E_0 decreases as $L^{-1/3}$, and R – increases as $L^{1/3}$.

Therefore, for each value of φ_0 from the dependence $E(n_0)$; $R(n_0)$ and $E(L)$; $R(L)$ the most optimal values of n_0 and L were determined, at which a higher efficiency of the nanoheterojunction is achieved.

Table 1

For example, with $\varphi_0 = 0.2$ V		
At $n_o = 2.5 \cdot 10^{22}$ m^{-3}	$E_o(n_o) = 4.22 \cdot 10^5$V/m	$R(n_o)$ = 0.947 μm
At $L = 10^{-4}$ m	$E_o(L) = 3.92 \cdot 10^5$V/m	$R(L)$ = 1.02 μm

These values of the strength, potential and length of the contact field, combined with the fact that the heterojunction is concentrated directly on the surface of the solar cell, make it possible to take into account minor recombination processes only in a relatively thin region of the space charge R.

The most optimal values of the surface density of nanoheterojunctions on the silicon surface at $n_0 = 2.5 \cdot 10^{22}$ m^{-3} is $8.55 \cdot 10^{10}$ cm^{-2}. This means that even with pico ampere photocurrents generated in each nanoheterojunction in macro solar panels, the total photocurrent generated will be quite large.

In addition, calculations have shown the possibility of reducing the thickness of the solar cell and bringing it to 80-100 microns without much loss of efficiency (unlike the current solar cells in use, the thickness of which is 200-450 microns).

3.3 Efficient Absorption of High-Frequency Photons in NCs PbX

One of the most important properties of solar panels is their operation only in the red and infrared spectra of sunlight, while the remaining spectra are scattered uselessly.

In conventional silicon solar cells, absorption of high-frequency photons generally only leads to heating and degraded efficiency. However, in a solar cell based on non-crystalline silicon and nanocrystals of lead chalcogenide, it is possible to effectively convert high-frequency components of solar radiation. This effect is possible due to the special properties of nanosized lead chalcogenides.

A separate section of a solar cell with many densely arranged nanoheterojunctions in a checkerboard pattern is shown in Fig. 4. One nanoheterojunction cell occupies area b_2, and the area of the nanoinclusion it-self occupies a_2. Light absorption occurs in both areas (b_2 and a_2), but in different ways: in b_2 – as in silicon ($0 < \hbar\omega < 1.7$ eV – maximum 26.5% of the solar radiation spectrum – "red light"), in a_2 – as in lead chalcogenides ($0 < \hbar\omega < 2.9$ eV – maximum 69.7% – "blue" light).

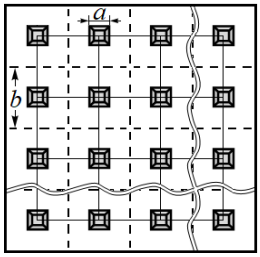


Fig. 4 – A single section of a solar cell with multiple densely packed nanoheterojunctions in a checkerboard pattern

In PbX with large quantum yields, the effects of MEG and CM are actively manifested, which causes the birth of a number of additional current carriers as a result of the absorption of one high-frequency photon.

The efficiency of the <Si:PbX> solar cell is largely determined by the ratio of the values: a and b. The greater the difference between a and b, the smaller the unique contribution of lead chalcogenides with characteristic manifestations of multiexciton generation and carrier multiplication. This conclusion follows from solving the problem of optimizing the studied value of solar cell efficiency depending on the parameters that determine its value.

An electron optically excited into the conduction band by a high-frequency photon very quickly radiatively relaxes within $10 \div 20$ *fs*.

Relaxation is accompanied by successive electron transitions to optically resolved lower multiexciton levels with the birth of a number of secondary low-frequency photons. The relaxation process continues until the initially generated electron loses almost completely the acquired energy.

Having passed into silicon, each secondary low-frequency photon gives birth to new current carriers and thereby increases the efficiency of the solar cell.

In accordance with the effect of multiexciton generation, secondary photons from one absorbed high-frequency photon in a nanosized crystalline lead chalcogenide are generated in an amount equal to the quantum yield.

4. CONCLUSION

The creation of a highly efficient solar cell based on non-crystalline silicon is possible in combination with nanocrystals of lead chalcogenide. Such solar cells can become new, promising devices for solar energy, which are almost impossible to create by other methods of combining contacting materials.

In nanocrystals, neither impact ionization nor intraband relaxation can compete in the speed of relaxation with the effect of carrier multiplication (they are strong only in macroscopic crystals). Due to its implementation, it is possible to significantly reduce energy losses associated with heating the solar cell.

The dependence of the efficiency of a solar cell on the properties of the materials of its components has been determined.

The features of the model for the formation of the contact field of the nanoheterojunction <Si:PbX> are shown.

The electrical parameters of the contact field of the nanoheterojunction <Si:PbX> are calculated, and the manifestation of the effect of multiexciton generation and the phenomenon of carrier multiplication are also considered. The effective absorption of high-frequency photons by nanocrystals of lead chalcogenide is considered.

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Дослідження електрофізичних процесів у кремнієвому сонячному елементі з багатьма поверхневими наногетеропереходами

M.A. Askarov[1,2], E.Z. Imamov[3], Kh.N. Karimov[3]

[1] *Karakalpak State University named after Berdakh, 230112, Nukus, Uzbekistan*
[2] *Tashkent Institute of Chemical Technology, 100011, Tashkent, Uzbekistan*
[3] *Tashkent University of Information Technologies named after Muhammad al-Khwarizmi, 100084, Tashkent, Uzbekistan*

На основі досліджень різних електричних проявів і властивостей некристалічного кремнію і кристалічних халькогенідів свинцю в нанорозмірному стані вперше зроблено висновок про мож-ливість створення на їх основі високоефективного сонячного елемента. Продемонстровано, що явища розмноження носіїв і генерації мультиекситонів відіграють значну роль у забезпеченні високої ефективності, завдяки чому можливе значне зниження втрат енергії, пов'язаних з нагріванням сонячного елемента. Визначено залежність ККД сонячного елемента від властиво-стей матеріалів його компонентів. Показано особливості формування контактного поля сонячного елемента та розраховано його електричні параметри. Розраховано внесок поглинання високоча-стотних фотонів в ефективність сонячної батареї.

Ключові слова: Енергія, Фотоелемент, Фотострум, Наногетероперехід, Структура, Некристалічний, Ефективність.