



REGULAR ARTICLE

Determination of Contact Field Parameters of a Solar Cell with Multiple Nanoheterojunctions <Si:PbX>

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Based on a non-standard choice of contact materials: non-crystalline silicon and nanosized crystalline lead chalcogenides (PbX), the possibilities of increasing the efficiency of solar cells by creating a solar cell with multiple nanoheterojunctions are substantiated. Based on the principle of self-organization, the possibilities of growing PbX nanocrystals in the form of coherent nanostructures on the surface of non-crystalline silicon are shown. The dependence of the solar cell efficiency on the properties of the materials of its components is determined. The features of the formation of the contact field of the solar cell are shown and its electrical parameters are calculated. The parameters of the contact field of the <Si:PbX> nanoheterojunction are calculated by solving the Poisson equation. The mechanism of contact field formation by equalizing the Fermi levels is explained, and the state of the final Fermi level is calculated. To determine the optimal parameters of the contact field of the nanoheterojunction, the number of electrons transferred from silicon to PbX was calculated. Calculations show that the parameters of the contact field of the nanoheterojunction <Si:PbX> are not inferior to similar parameters of conventional silicon solar cells.

Keywords: Solar cell, Silicon, Nanoheterojunction <Si:PbX>, Lead chalcogenides, Non-Crystalline, Efficiency.

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1. INTRODUCTION

Many energy crises in recent years have led people to realize the urgent need to search for new energy sources to replace the gradually depleting reserves of hydrocarbons. Naturally, renewable energy sources (RES), including solar energy, are at the forefront of this search.

The potential of solar energy is indeed impressive due to its inexhaustibility, which, unfortunately, cannot be said about the current practical capabilities of harnessing it. The main issue lies in the low efficiency of solar panels, along with a number of operational challenges in using solar electricity. As a result, this issue has attracted the attention of many researchers.

The efficiency of a solar panel is primarily determined by its main component – the solar cell (SC), and more specifically, by the properties of its p-n junction, where the conversion of solar radiation into electricity takes place.

The solar cell (SC), as the fundamental component of solar energy systems, is largely responsible for their efficiency. More precisely, the efficiency of an SC is determined by the conversion properties of its p-n junction, which depend on the choice of contacting

materials: when the materials are identical, the junction is a homojunction; if the materials are different, it is a heterojunction.

This study examines the properties of a SC composed of a unique and entirely unconventional combination of contacting materials for solar energy applications: amorphous non-crystalline silicon (Si) combined with numerous nanoinclusions of lead chalcogenide semiconductors (PbX, where X = S, Se, Te).

The unconventional nature of this SC lies not only in the rather "unusual" combination of materials but also in its application within solar panels for the large-scale production of solar electricity. These panels must retain their conversion efficiency while operating over extended periods in open environments with extreme fluctuations in climatic conditions. Therefore, a thorough justification is required for the SC's long-term operational stability, specifically the need to:

- provide a detailed rationale for the choice of contacting materials (Si and PbX);
- justify the manufacturing technology necessary for producing such a complex solar cell that retains stable conversion performance over years of use;

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- substantiate the mutual compatibility of the contacting materials (Si and PbX).

At present, high efficiency in solar cells is achieved primarily through the use of monocrystalline silicon as the base material (or, at minimum, polycrystalline silicon). The idea of using amorphous, non-crystalline silicon as one of the contacting materials in a solar cell – while expecting high efficiency – has long been regarded as entirely unpromising, if not outright meaningless.

However, contrary to these negative expectations, a number of experimentally confirmed and patented properties have demonstrated that it is indeed possible to create efficient energy conversion devices based on the combination of amorphous silicon and lead chalcogenide (PbX) nanocrystals [1-5].

The conclusion that efficient conversion devices can be developed from these two non-traditional materials – Si and PbX – whose contact can provide a solar cell with long-term, stable energy conversion efficiency, necessitates a thorough investigation of the physics of each SC material and the formation process of the heterojunction between them.

We begin with an individual analysis of each component. We aim to determine the extent to which the unique optical and electrophysical properties of amorphous silicon and lead chalcogenide nanocrystals can contribute to the formation of a nanoheterojunction <Si:PbX>.

2. FORMATION OF THE CONTACT FIELD OF A NANOHETEROJUNCTION <SI:PBX>

The formation of the contact field is accompanied by transitions of N electrons from Si to PbX ($F_{Si} > F_{PbX}$). They cease when the Fermi levels become equal, at which the contact potential

$$\varphi_0 = \frac{F_{Si} - F_{PbX}}{e}$$

According to the theory of fluidity, the occurrence of a directed flow of particles between two volumes occurs from a material with a higher W – volumetric energy density (dimension J/m^3) to a lower W .

Further, the beginning of the energy count is transferred to the position $F_{PbX} = 0$. In this case (see Fig. 1), the initial energy of all N electrons moving from Si to PbX is equal to: $F_{Si} = q\varphi_0$.

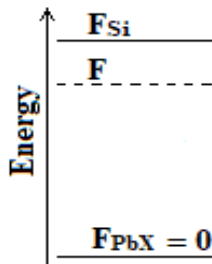


Fig. 1 – Fermi level alignment

The complete formation of the contact field is accompanied by:

- the flow of electrons into the nanocrystal (PbX) due to some part of the volumetric energy density of silicon, equal to

$$W = \frac{F_{Si} - F}{\varepsilon_{Si} R b_0^2}$$

- an increase by the same value of

$$W = \frac{F}{\varepsilon_{PbX} a^2 d}$$

– the volumetric energy density in the PbX nanocrystal due to the influx of N energy-saturated electrons from silicon;

- the establishment of an equilibrium state of the entire nanoheterojunction with a single final energy level F .

Contact field of a nanoheterojunction. By analogy with the theory of a semiconductor thin p - n junction [6-11], the contact field of a nanoheterojunction <Si:PbX> is calculated. Integration of the one-dimensional Poisson Eq.:

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

determines the magnitude of the electric field strength vector $E(x)$ of the contact field and its potential $\varphi(x)$. For $\varphi(x)$ and $d\varphi/dx$, taking into account the boundary conditions and continuity conditions, the solutions $E(x)$ and $\varphi(x)$ of the Poisson equation (in the interval $0 < x < R$ and with ρ – the space charge density) have the form:

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

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

The amplitude values (at $x=0$) of the contact field parameters (E_0 – the modulus of the field strength vector and φ_0 – the potential difference) at the end of the process of nanoheterojunction formation are equal to:

$$E_0 = \frac{\rho R}{\varepsilon_{Si}\varepsilon_0} \quad \text{and} \quad \varphi_0 = -\frac{\rho R^2}{2\varepsilon_{Si}\varepsilon_0} \quad (3)$$

The final potential difference of the contact field (or the amplitude value

$$\varphi_0 = \frac{1}{2} E_0 R,$$

established at the end of the process of nanoheterojunction formation, is determined by the difference in the equilibrium values of the Fermi energies of the initial materials (Si and PbX):

$$\varphi_0 = \frac{F_{Si} - F_{PbX}}{e}.$$

The length of the contact field $R = Nb_0$ is determined by N , the number of electrons whose transition from Si to PbX forms the contact field, and b_0 , the average length of chaotic thermal jumps of an electron, which is also the average distance between adjacent local defect energy states (LDES) in the for-bidden band of Si (see Fig. 2).

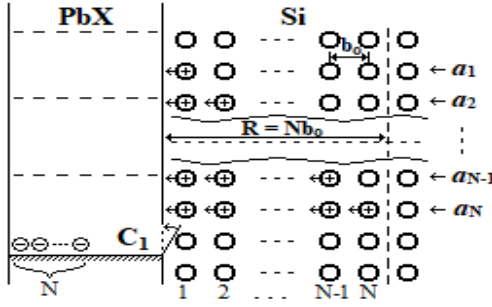


Fig. 2 – Band diagram of the formed nanoheterojunction <Si:PbX>

Considering a nanocrystal PbX in the form of a flat plate of thickness d and area a^2 , according to the Gauss theorem for a conducting and charged ($q = eN$) plane, at the end of the process of formation of the nanoheterojunction, the values of E_0 and φ_0 will take the form:

$$E_0 = \frac{q}{2\varepsilon_{PbX}\varepsilon_0 a^2} \quad \text{and} \quad \varphi_0 = \frac{qR}{4\varepsilon_{PbX}\varepsilon_0 a^2} \quad (4)$$

Here ε_0 is the permittivity, and ε_{Si} and ε_{PbX} are the

permittivities of Si and PbX. The volume charge density

$$\rho = \frac{q}{Rb_0^2}$$

is formed due to transitions of N electrons (electrons or holes depending on the ratio of the initial values F_{Si} and F_{PbX} , it is further assumed that $F_{Si} > F_{PbX}$) from LDES in Si into the nanocrystal. The space charge region in Si has the shape of a parallelepiped with a square base a^2 and a height R . The base a^2 is located in the center b^2 , adjacent to the nanocrystal of the illuminated square surface of silicon. The spatial distances between the charged LDES (neutrality is violated by the transition of electrons in PbX), which form the contact field of the nanoheterojunction in silicon, determine the sides b and b_0 : b is the distance between two surface crystallites ($n_\Sigma = b^{-3}$ is their surface concentration); b_0 is the distance between two bulk crystallites ($n_\Omega = b_0^{-3}$ is their volume concentration). The geometric shape of the nanoheterojunction in Si has the form of two squares inserted into each other at the center: b_0^2 in-side b^2 ($b > b_0$ – see the Fig. 3). The volume of the contact field in the form of a parallelepiped is equal to Rb_0^2 .

For the convenience of discussing the problem, we will introduce some dimensionless coefficients, the values of which will characterize the parameters of the nanoheterojunction <Si:PbX>:

$$k = \frac{b}{a}, \quad \alpha = \frac{b_0}{b}, \quad \varepsilon^* = \frac{\varepsilon_{Si}}{\varepsilon_{PbX}}, \quad z = \frac{a}{d}$$

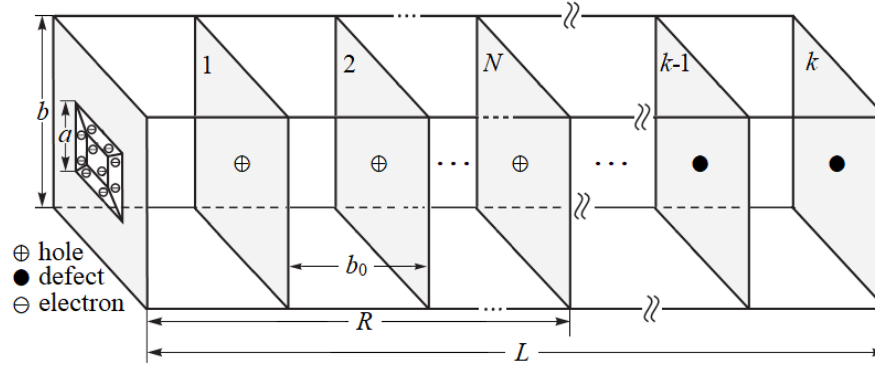


Fig. 3 – Formation of the contact field of the nanoheterojunction <Si:PbX>

By comparing two correct relationships (3) and (4) for the amplitude value of the electric field strength E_0 , we find the number of electrons N , the transition of which from Si to PbX forms the final value of the contact field of the nanoheterojunction. Indeed, taking into account the relationships

$$E_0 = \frac{2\varphi_0}{R}, \quad b_0 = \alpha ak, \quad q = eN, \quad R = Nb_0, \quad k = \frac{b}{a},$$

$$\varphi_0 = \frac{F_{Si} - F_{PbX}}{e}$$

we can obtain:

$$N = \left(\frac{4\varphi_0 \alpha \varepsilon_{PbX} \varepsilon_0}{e a k} \right)^{\frac{1}{2}} \quad (5)$$

From this relation it is evident that the number of electrons N is essentially determined by the parameters of

the nanoheterojunction materials, i.e. Si and PbX. F_{Si} , F_{PbX} , α , α , k . Knowing φ_0 , and also assuming that F_{Si} , F_{PbX} , ε^* , k , α , z are given (i.e. considering them to be known a priori), using the calculated N (5) all the parameters of the contact field of the nanoheterojunction <Si:PbX> are found:

- $N(\varphi_0)$ is the number of electron transitions from Si to PbX;
- $E_0(\varphi_0)$ is the amplitude of the modulus of the electric field vector;
- $q(N(\varphi_0))$ is the number of electrons on the surface (α^2) of the nanocrystal;
- $R(N(\varphi_0))$ is the length of the space charge region in silicon;
- F – equilibrium Fermi level in the formed nanoheterojunction.

3. RESULTS AND ITS DISCUSSION

As noted above, to determine the most optimal parameters of the contact field of the nanoheterojunction, it is necessary to know N – the number of electrons transferred to PbX from silicon. It is determined by the amount of work per unit volume to form the potential φ_0 . In our case, this is the volumetric energy density of silicon. It is spent on two types of work:

- The first part A_k – on the work of "shifting" the electron from the initially neutral LDES to the adjacent free defect level (or "push" to detach the electron from the neutral defect and give it speed). Using Coulomb's law, the value of A_k is defined as:

$$A_k = \frac{e\varphi_0 N}{2Rb_0^2} = \frac{e^2}{4\pi\varepsilon_{Si}^2\varepsilon_0\alpha^4 k^4} \quad (6)$$

- The second A_r is the fraction of the volumetric energy density spent on the work of overcoming the electrical resistance of the silicon medium by the electron (on the way to contact with the PbX nanocrystal). Using the Joule-Lenz law, the value of A_r is defined as:

$$A_r = \frac{I^2 R t}{\varepsilon_{Si} N b_0^3 \alpha^2 \sigma} = \frac{1}{3} \varepsilon^* \pi (2N^2 - 3N + 1) \cdot A_k \quad (7)$$

From the above follows the equality:

$$\frac{F}{\varepsilon_{PbX} \alpha^2 d} = \frac{F_{Si} - F}{\varepsilon_{Si} R b_0^2},$$

which allows us to determine F – the value of the energy level finally established for the entire nanoheterojunction:

$$F = \frac{F_{Si}}{1 + \gamma} = \frac{q\varphi_0}{1 + \gamma}, \quad (8)$$

where

$$\gamma = \frac{\varepsilon_{Si} R b_0^2}{\varepsilon_{PbX} \alpha^2 d} = \frac{\alpha k^3 z N}{\varepsilon^*}$$

Thus, as a result of the work on transferring N

electrons from silicon to PbX, the volumetric energy density of silicon decreased by the value

$$A = A_k + A_r = \left[1 + \frac{1}{3} \varepsilon^* \pi (2N^2 - 3N + 1) \right] \cdot A_k \quad (9)$$

The volumetric energy density of the lead chalcogenide nanocrystal increased by the same amount. By equating them and assuming

$$\frac{\gamma}{1 + \gamma} = y,$$

we obtain an equation for determining N , taking into account changes in the values of the volumetric energy densities of the lead chalcogenide nanocrystal and non-crystalline silicon:

$$N = \frac{3 + \varepsilon^* \pi (2N^2 - 3N + 1)}{3\pi\varepsilon^* \alpha^2 k^2} \cdot y \quad (10)$$

At first glance, a rather complex equation was obtained for the number of electrons. However, if

$$\frac{\gamma}{1 + \gamma} = y$$

is set almost equal to unity (since γ is the ratio of the volumetric energy densities of silicon and the lead chalcogenide nanocrystal is significantly greater than unity), then with such simplification (10) is reduced to a quadratic equation with respect to N :

$$2N^2 - 3N \left(1 + y \alpha^2 k^2 \right) + \frac{3}{\varepsilon^* \pi} + 1 = 0 \quad (10^*)$$

The found number of electrons N , forming the contact field of the nanoheterojunction, depends mainly on three parameters: α , k and ε^* . For example, at

$$\alpha = \frac{b_0}{b} = \frac{2}{3}, \quad k = \frac{b}{a} = 3, \quad \varepsilon^* = \frac{\varepsilon_{Si}}{\varepsilon_{PbX}} = \frac{12}{176}$$

the value of $N = 7$. And this means that at $\varphi_0 = 0.2$ V and $N = 7$:

- length of the contact field in silicon: $R(N(\varphi_0)) = 7 \cdot 20/3 = 46$ nm;
- on the surface of 11 nm² the number of electrons: $q(N(\varphi_0)) = 7$ e;
- amplitude of the electric field strength: $E_0(\varphi_0) = 9 \cdot 10^6$ V/m;
- Fermi level in the formed nanoheterojunction: $F = 0.03$ eV.

As noted above, to determine the most optimal parameters of the contact field of the nanoheterojunction, it is necessary to know the number of electrons transferred to PbX:

$$N = \frac{3 + \varepsilon^* \pi (2N^2 - 3N + 1)}{3\pi \varepsilon^* \alpha^2 k^2} \cdot y.$$

Variation (5) or (10) by k , α and z allows us to determine the most optimal parameters of the nanoheterojunction and the corresponding physical conditions for converting solar radiation into electricity.

4. CONCLUSION

Innovative choice of contacting materials of the solar cell (nanosized crystalline lead chalcogenide and structureless non-crystalline cheap silicon) determines its efficiency.

Significant improvement of the converting properties of the solar cell is achieved by the detailed specific

electrophysical properties of PbX and Si.

Creation of a highly efficient solar cell based on non-crystalline silicon is possible in combination with lead chalcogenide nanocrystals.

Such solar cells can become new, promising devices for solar energy, which are almost impossible to create by other methods of combining contacting materials.

The dependence of the solar cell efficiency on the properties of the materials of its components is determined.

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

Electrical parameters of the contact field of the nanoheterojunction <Si:PbX> are calculated. Also, the number of electrons forming the nanoheterojunction is calculated.

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Визначення параметрів контактного поля сонячного елемента з кількома наногетеропереходами <Si:PbX>

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На основі нестандартного вибору контактних матеріалів: некристалічного кремнію та нанорозмірних кристалічних халькогенідів свинцю (PbX), обґрунтовано можливості підвищення ефективності сонячних елементів шляхом створення сонячного елемента з кількома наногетеропереходами. На основі принципу самоорганізації показано можливості вирощування нанокристалів PbX у вигляді когерентних наноструктур на поверхні некристалічного кремнію. Визначено залежність ефективності сонячного елемента від властивостей матеріалів його компонентів. Показано особливості формування контактного поля сонячного елемента та розраховано його електричні параметри. Параметри контактного поля наногетеропереходу <Si:PbX> розраховано шляхом розв'язання рівняння Пуассона. Пояснено механізм формування контактного поля шляхом вирівнювання рівнів Фермі та розраховано стан кінцевого рівня Фермі. Для визначення оптимальних параметрів контактного поля наногетеропереходу було розраховано кількість електронів, що переносяться з кремнію на PbX. Розрахунки показують, що параметри контактного поля наногетеропереходу <Si:PbX> не поступаються аналогічним параметрам звичайних сонячних кремнієвих елементів.

Ключові слова: Сонячний елемент, Кремній, Наногетероперехід <Si:PbX>, Халькогеніди свинцю, Некристалічний, Ефективність.