FORMATION OF A SOLAR CELL BASED ON NANO HETERO JUNCTIONS

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Abstract. *The paper solves the problem of increasing the efficiency of a solar cell based on a combination of two technologies: nano technology and technology for creating semiconductor hetero junctions. It is shown that the use of three types of nano-crystals of lead chalcogenides: PbS, PbSe, PbTe contribute to increasing the efficiency of the solar cell. A zone diagram of the nano hetero transition is constructed PbS:Si, by analogy with the construction of a zone diagram of a macroscopic hetero junction. When analyzing the construction of the band diagram, a significant dependence of the density of the linear multi-exciton energy spectrum of electrons and holes in nanocrystals on the ratio of their effective masses is taken into account.*

Keywords: *solar cell, lead chalcogenides, nano hetero junction, zone diagram, carrier multiplication.*

Introduction. Many energy collapses of recent years have led people to think about the urgent need to find new sources of energy to replace the gradually disappearing hydrocarbon reserves. Naturally, at the same time, RES - renewable energy sources, including solar energy, are in the first positions.

The possibilities of solar energy are really impressive in their inexhaustibility, which cannot be said about the current applied cases of its development. The main problem is the low efficiency of solar panels and a number of operational problems with the use of solar electricity.

One of the numerous approaches to the problem of increasing the efficiency of a solar cell is to study the problem in combination with two technologies: nano technology and technology for creating semiconductor hetero junctions. The possibilities of nano-technology are considered due to the fact that a solar cell (with a silicon substrate) contains a large number of nano-dimensional components (*the above concerns nano crystals with sizes approaching the size of an atom - on the order of several nanometers*) and has expanded functionality based on new principles and new manifestations of known physical phenomena in semiconductor materials [1-3]. In particular, due to the significant transformation of optical phenomena in a solar cell by reducing the size of its nano-structural components, a certain improvement in the efficiency of solar conversion is considered in the work (dimensional limitations in the nature of electron motion in nano crystals leads to changes in its electronic, optical, acoustic and other properties).

The use of the capabilities of semiconductor hetero junction technologies is investigated due to the fact that the solar cell considered in the work is a complex structurally modified structure. In it, a single solar cell (p-n junction) is replaced by a complex hetero junction device in which many (*by one* cm^2 $8 \cdot 10^7$ *and more [1]*) nano crystals (NC) from another p-type semiconductor are created on the surface of a silicon substrate (say n-type), followed by the formation of nano-dimensional hetero junctions (or nano hetero junctions - NHJ) in them (PbX:Si). A particularly noticeable improvement in the efficiency of the solar cell is achieved when using lead chalcogenides (PbX: PbS, PbSe, PbTe) as a material of nano crystals, which led to a more detailed description of the properties of PbX - lead chalcogenides.

Properties of nano crystals PbX. Three types of nano crystals of PbX - lead chalcogenides are investigated: PbS, PbSe, PbTe. They have three unique properties.

The first feature is that as the transverse dimensions of a nano crystal increase (up to 20-30 nm), the width of its multi–exciton energy levels increases significantly due to the Coulomb interaction. As noted in [4], for spherical nano particles with radius R, the increase is proportional to R^{-1}. At the same time, the width between the last electron-filled level of the nano crystal (analog of the valence band) and its first empty level (analog of the conduction band) also increases, that is, the analog of the band gap width in the macrocrystal of lead chalcogenide E_g^{PbX} increases.

The second feature is that changing the size and width of multi-exciton energy levels in nano crystals of lead chalcogenides leads to rapid (10-20 fs) radiation recombination of an electron generated during their absorption of a high-energy photon. The resulting series of low-energy photons, penetrating deep into the silicon substrate, are absorbed in them and are able to generate new electron-hole pairs (that is, they cause the phenomenon of carrier multiplication [5]). This can lead to a multiple increase in the contribution of the nano-crystalline component of the solar cell to the efficiency of light conversion [2].

The third feature of nano crystals of lead chalcogenides is that their growth is most favorably realized by the process of self-organization in those areas of the substrate where PbX nano crystals with a high value of dielectric permittivity naturally find areas of crystalline compatibility with silicon [6]. On these areas of the silicon substrate surface, nano crystals of lead chalcogenides form a set of nano PbX:Si hetero junctions.

Zone diagrams of NHJ PbX:Si. The study of the mechanisms of light transformation in nano-hetero transitions based on PbS is carried out on the basis of consideration (*macro hetero junction PbS:Si is built on the basis of data [7]: PbS - electronic affinity* $\chi = 4.35$ *eV, output operation* $F = 4.66$*eV,* $E_g = 0.41$*eV (300 K), permittivity = 175, lattice constant = 5.94 Å; Si - electron affinity* $\chi = 4.01$ *eV, output operation* $F = 4.41$*eV,* $E_g = 1.08$*eV (300 K), permittivity = 12, lattice constant = 5.43 Å*) of their zone diagrams, which are constructed according to the same rules as the zone diagram of macroscopic hetero junction PbS:Si (Fig.1-a [7]). At the same time, the zone of the substrate - macro-dimensional silicon practically does not change, and the zones of nano–dimensional lead chalcogenides PbS (Fig.1-b) - have been completely updated: continuous energy zones have been replaced by a linear series of multi-exciton energy levels. The width of the discrete levels between the series of linear multi-exciton energy levels of holes and electrons is the same, since they have approximately equal effective masses ($m_p \approx m_n$). In nano-sized lead chalcogenides, with a decrease in their size, the E_g^{PbS} increases - the width of the zone between the last electron-filled state and the first empty one (Fig.1-b).

This shows the peculiarity of the linear multi-exciton energy spectrum in PbX nano crystals in contrast to the spectrum of nano crystals of other semiconductor materials. For example [3], CdSe due to the strong difference between the effective masses of electrons and holes ($m_p >> m_n$), where the density of linear multi-exciton energy levels of holes is much denser than that of electronic states (Fig.1-c, constructed by analogy with Fig.1-b).

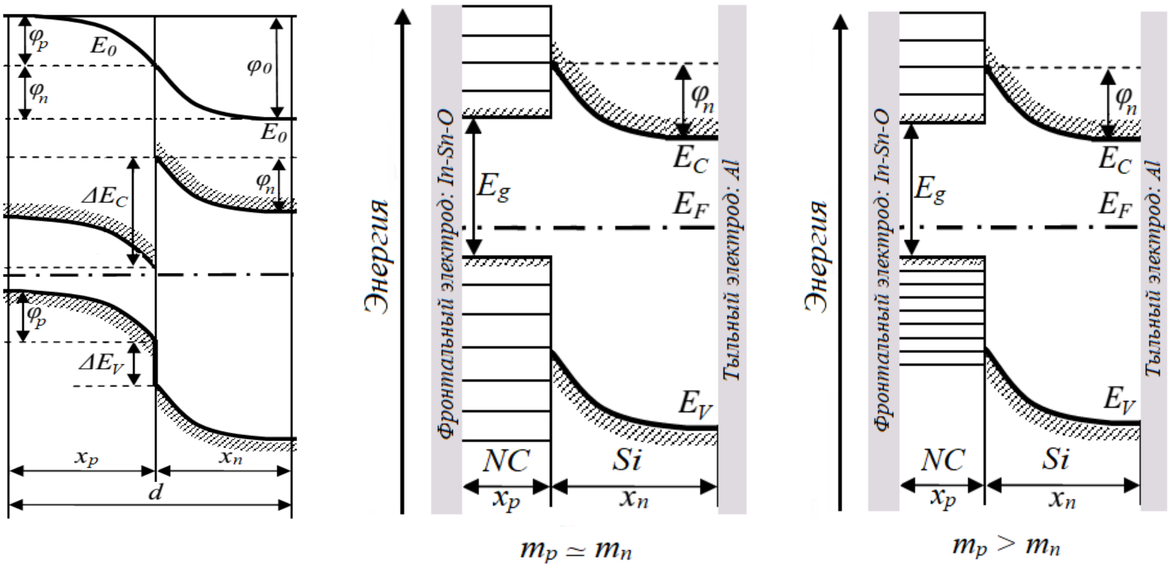

Fig.1-a: macro hetero junction **PbS:Si**

Fig.1-b: nano hetero junction **PbS:Si**

Fig.1-c: nano hetero junction **CdSe:Si**

The contribution of the shock ionization phenomenon to the process of light transformation in nanocrystals. The efficient conversion of solar energy into electricity is accompanied by the absorption of a single photon in a semiconductor, followed by the birth of one electron-hole pair. In this case, the internal quantum output is equal to one (one photon generates one electron-hole pair).

Higher values of the quantum yield are characteristic under the condition of the realization of the so-called carrier multiplication (CM) phenomenon associated with shock ionization [2, 8-12]. However, the observation of the CM phenomenon in bulk semiconductors is very difficult [12] due to the contentedly strong competition of another phenomenon – the transient intraband relaxation of carriers. It is this non-radiation relaxation that prevents CM in a bulk semiconductor and does not allow us to observe the phenomenon of an increase in the quantum yield, when one photon can give birth to several electron-hole pairs.

A completely different situation with the CM process is observed in ultra-small semiconductor nano crystals, in particular, the CM process is especially strongly manifested in nano crystals made of lead chalcogenides PbX: PbS, PbSe, PbTe [2]. In these quantum-limited semiconductors, CM becomes a very efficient process, accompanied by the generation of several electron-hole pairs when one high-energy ($\hbar\omega >> E_g^{PbX}$) photon is absorbed, which makes it possible to use CM in processes related to the functioning of solar converters with nano cluster inclusions [2,12]. For example, generation of four electron-hole pairs was observed in PbS nano crystals, and even seven in PbSe [13, 14].

Such large values of quantum yields can contribute to improving the efficiency of solar cells with NHJ PbX:Si. Such an improvement in efficiency is due to the absorption of low-energy photons ($\hbar\omega < E_g$) generated in the process of multiplication of carriers in silicon.

Usually, the absorption of high-energy photons only leads to heating of the solar cell and a significant deterioration in its efficiency of converting light into electricity. However, due to the implementation of the CM effect, in nano-hetero PbX junctions: Si the efficiency of the solar cell will only increase, that is, it can be stated that semiconductor nanocrystals "are promising materials for creating inexpensive and highly efficient photovoltaic systems", as well as solar panels "based on silicon [14]. In addition, it is stated in [14] that the SI effect is able to significantly reduce the heating losses of a solar cell from 90 percent to 10 percent in the processes of converting light into electricity.

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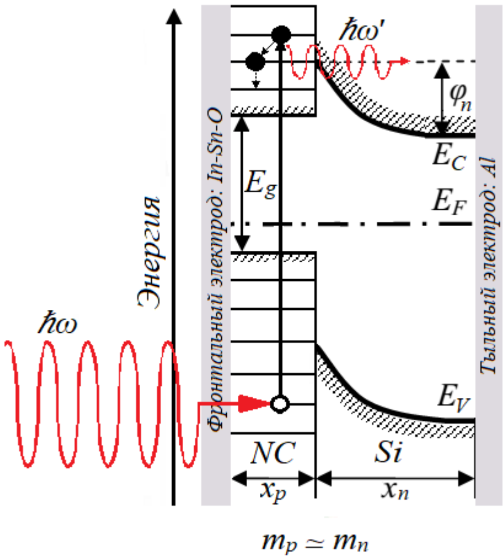

Fig. 2: Nano hetero junction **PbS:Si** as a solar radiation converter on an arbitrary energy scale.

Based on the model of formation of NHJ PbX:Si (Fig.1–b), the physics of the CM effect is considered. Figure 2 shows the process of interaction of high-energy radiation with NHJ PbX:Si. The high-frequency photon ħω of solar radiation falls on the NHJ, and the second-born low-frequency photons ħω' are directed and absorbed in silicon with the birth of many new electron-hole pairs.

The absorption of a high-frequency photon (ħω) is accompanied by the birth of an electron–hole pair, the electron of which reaches the upper level of the multi-exciton discrete states of the analog of the conduction band, and the hole occupies the lower level of the multi-exciton discrete states of the analog of the valence band.

In nano-sized lead chalcogenide, the transition of an excited electron from the nth to the (n - 1) level of a linear series of multi-exciton energy states is accompanied by the emission of a ħω' - secondary photon, which, passing into silicon, causes a new generation of an electron-hole pair due to its impurity or interband absorption, that is, the Auger effect is realized - generation.

In turn, an electron trapped at the (n - 1) th level can move to the (n - 2) th lower multi-exciton level with the birth of a second low-frequency photon of the infrared region of solar radiation ħω'. And so the process in NHJ PbS:Si can continue until the initially generated electron loses almost all of its acquired energy, that is, after the generation of 4 electron-hole pairs. These 4 electron-hole pairs concentrated in silicon will contribute to the process of converting light radiation into electricity. This contribution became possible precisely due to the absorption of high-frequency photons, which previously only heated the solar cell.

This is the essence of the CM effect, which a solar cell with many NHJs is able to noticeably expand the spectrum of effective absorption of solar radiation.

Conclusion. The problem of increasing the efficiency of the solar cell is solved in the work on the basis of a combination of two technologies: nano technology and technology for creating semiconductor hetero junctions.

It is shown that the use of three types of nano-crystals of lead chalcogenides: PbS, PbSe, PbTe contribute to increasing the efficiency of the solar cell.

A zone diagram of the nano hetero junction PbS is constructed PbS:Si, by analogy with the construction of a zone diagram of a macroscopic hetero junction.

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