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Properties of lead chalcogenide nanocrystals in nanoheterojunctions <Si:PbX>

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Аннотация. Рассмотрен вопрос об использовании некристаллического кремния в качестве подложки эффективного солнечного элемента. Показано, что создание эффективного солнечного элемента из некристаллического кремния возможно только при больших плотностях локализованных дефектных энергетических состояний в глубине запрещенной зоны кремния. Показано, что особенно эффективное преобразование солнечной энергии в электричество возможно при сочетании в качестве компонентов гетеропереходов двух материалов: некристаллического кремния и халкогенидов свинца в нано размерном состоянии. Показано, что особенно халкогенидам свинца свойственны сильное проявление эффектов мульти-экситонной генерации и умножения носителей.

Ключевые слова: Солнечный элемент, эффективность, наногетеропереход, мультиэкситонная генерация, умножение носителей.

Annotation. The question of using non-crystalline silicon as a substrate of an effective solar cell is considered. It is shown that the creation of an effective solar cell from non-crystalline silicon is possible only at high densities of localized defective energy states in the depth of the silicon band gap. It is shown that a particularly effective conversion of solar energy into electricity is possible when two materials are combined as components of heterojunctions: non-crystalline silicon and lead chalcogenides in the nano-dimensional state. It is shown that especially lead chalcogenides are characterized by a strong manifestation of the effects of multi-exciton generation and carrier multiplication.

Key words: Solar cell, efficiency, nanoheterojunction, multi-exciton generation, carrier multiplication.

1. INTRODUCTION

The efficiency of solar energy is mainly determined by its main primary component – the solar cell (SC), or rather, the efficiency of the transforming property of its *p–n* junction. The latter, in turn, depends on the choice of contacting materials.

We consider a special unconventional situation of combining structureless non–crystalline silicon with a nano-sized crystalline semiconductor of lead chalcogenide - PbX (X can be S; Se; Te) as a second material that creates a rectifying contact field (or *p-n* heterojunction).

Earlier in [1-20], various aspects of the possibility of creating converting devices based on two non-traditional materials (structureless non-crystalline silicon and a nano-sized crystalline semiconductor of lead chalcogenide) were considered. The contact between them is able to provide a sufficiently efficient solar cell that has been steadily preserving its transformative qualities for years.

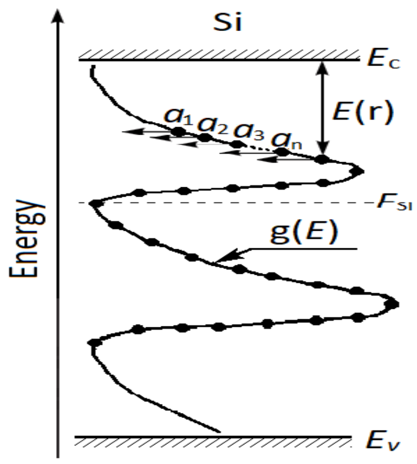
This article investigates the physical processes on the basis of which such a non-traditional combination of materials leads to the formation of a nanoheterojunction (NHJ) based on them <Si:PbX>. The results of studies of peculiar optical and electrophysical properties are presented below separately for each of them.

2. MATERIALS AND METHODS

2.1. Non-crystalline structureless silicon in a solar cell

Any solid body, including non-crystalline silicon, contains a certain number of various foreign bodies: structural defects, interstitial vacancy atoms, lattice imperfections, etc. Fig.1 (hereinafter we will call them defects). In the energy band spectrum of silicon, all these foreign additions are determined by

(Fig. 1)



(Fig. 1)

their discrete levels. If they are located in the permitted zones, then these are the so–called delocalized energy states, and if in the forbidden zone - localized defective energy states (LDES).

The wave functions of carriers at defective levels are concentrated near the corresponding defect and are characterized by energies E_i and spatial location at points r_i. Their energy density is equal to g(E), where E(r) is the value of the binding energy of the defect to the conduction band. Figure 1 shows a diagram of the location of localized defective energy states on a continuous curve g(E) - the density of states in the form of discrete points a_i (where i runs through values from 1 to n). In structureless non-crystalline silicon, the concentration of localized defective energy states is high (on the order of $10^{24}\div10^{26}$ m^{-3}) [21] and partially (or completely) cover uniformly the entire band gap, possessing both donor (above the Fermi level) and acceptor properties (below – acceptor). From levels a_1, a_2, a_3, ..., a_n, electrons in contact with nanocrystalline lead chalcogenide PbX pass to its multi-exciton levels. These transitions are implemented only when the corresponding levels coincide.

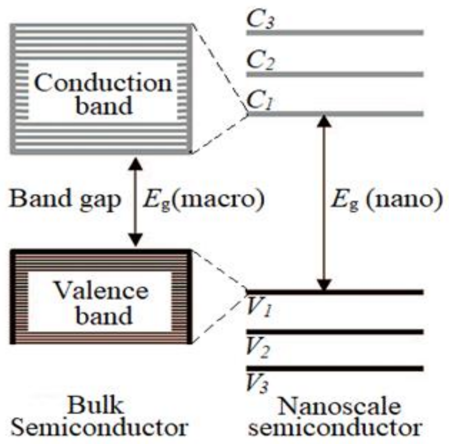
For a localized defective energy state of a_{n+1}, the arrow shows the value of its binding energy E(r) to the bottom of the conduction band. The level a_i (E_i and r_i) is located at a distance of $\rho = (r_{i+1} - r_i)$ from the neighboring level a_{i+1} (E_{i+1} and r_{i+1}). Here ρ - characterizes the radius of a localized electron averaged over all defective states of the band gap.

2.2. Nanoscale crystalline lead chalcogenides in a solar cell

Consideration of the second component of the solar cell concerns exclusively nanoscale crystalline lead chalcogenides, as well as their individual peculiar optical and electrophysical properties, providing a significant improvement in the transformative properties of the solar cell.

Nano crystals of lead chalcogenides in the form of separate "islands" in accordance with the principle of self-organization of matter [22-25] are formed on the surface of non-crystalline silicon by molecular beam epitaxy (MBE) [26,27].

In nanoscale crystals of lead chalcogenides, the energy zones of the allowed electron states are strongly deformed and are represented as narrow energy zones. They are so narrow that they resemble discrete levels of a single atom



(Fig. 2).

The dashed lines in the figure demonstrate how a wide energy conduction band turns into a narrow single "quasi-level" C_1 (and the valence band into a "quasi-level" V_1). The density of quasi-levels is inversely proportional to the geometric size of the nanocrystal.

Due to the approximate equality of the effective masses of current carriers in the "valence band" and in the "conduction band" ($m_p \approx m_n$), the distance between the "quasi-levels" in both zones is almost the same [23]. Their values are inversely proportional to the geometric size of the nanocrystal.

The peculiarity of nanoscale crystals of lead chalcogenides is that the width of the "forbidden zone" does not decrease, but increases with a decrease in their dimensions. For example, E_g^{PbS} at 300K is equal to 0.4 eV, and in nano-sized PbS increases by 1.3-2 times [23].

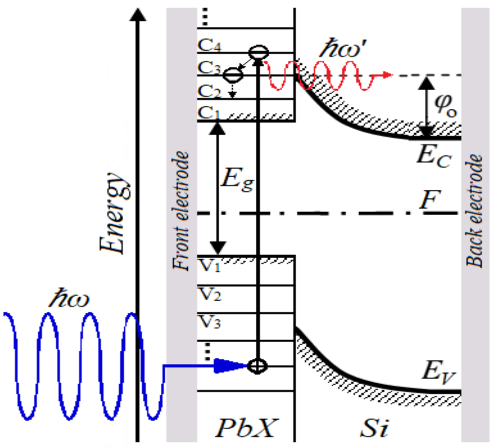
An important distinguishing feature of lead chalcogenides is an extremely high value of static dielectric permittivity: at 77 K: $\varepsilon_{PbS}= 178\div184$, $\varepsilon_{PbSe} = 227$, $\varepsilon_{PbTe}=1300$ [28]. The relatively large values of their static permittivity follow from the ionic nature of the interactions of atoms in their crystal lattices [29].

2.3. Optical and electrophysical properties of PbX

The paper considers some peculiar optical and electrophysical properties of PbX. They can provide an improvement in the transformative properties of the resulting nanoheterojunctions <Si:PbX> (nanoheterojunctions between Si and PbX).

PbX nano crystals in the form of "islands" are formed on the surface of non-crystalline Si by molecular beam epitaxy (MBE) in accordance with the phenomenon of self-organization [30-34].

The main attractive side of PbX nano crystals is that two phenomena are especially strongly manifested in them at the same time: MEG – multiexciton generation [23] and MC - multiplication of carriers [24]. When a high-frequency photon is absorbed in PbX due to multiexciton generation, n secondary photons are born, which, passing into Si, give birth to n new current carriers due to multiplication of carriers



(Fig.3).

The appearance of n secondary electrons in Si will make an additional contribution to the process of converting light radiation into electricity, that is, high-frequency photons are involved in the production of electricity. Without multiexciton generation and multiplication of carriers phenomena, absorption of high-frequency photons in a nanoheterojunctions <Si:PbX> usually led only to heating and deterioration of the efficiency of the solar cell.

3. RESULTS AND DISCUSSION

Light absorption in PbS. Light electricity is determined by the process of light absorption in "a^2" of the illuminated surface of the nanoheterojunctions <Si:PbS>.

If $\hbar\omega >> E_g^{PbS}$, then in PbS light absorption is accompanied by the manifestation of large values of the quantum yield β. If $\hbar\omega > E_g^{PbX}$, then one quantum effect works in this case. For example, the table shows 4 frequency ranges for PbS with different β (β varies from 1 to 4) [22,35].

The calculation of the total amount of effectively absorbed photons by the surface of the "a^2" nanoheterojunction requires determining the N_i^{PbS} - the number of effectively absorbed photons in each i-band β. For this, the peak intensity of solar radiation in Uzbekistan (900 W/m^2) is multiplied sequentially by β and "a^2", then divided by the average photon energies in the corresponding i -range [6]). As a result, the full nanoheterojunctions ratio is obtained:

$$N_{PbS} = \Sigma N^i_{PbS} = 5{,}19\cdot10^{22}\cdot a^2.$$

In the silicon region of nanoheterojunctions <PbS:Si> the number of effectively absorbed N_{Si} photons is characterized by a limited spectrum of effective light absorption (in Si it is 1.0 – 1.7 eV) on the area "b^2 - a^2" ("b^2" is the average area of Si adjacent to one PbS nanocrystal):

$$N_{Si} = 2{,}75\cdot10^{21}\cdot(b^2 - a^2).$$

Ranges of manifestation of MC and MEG effects in PbS nanoinclusions

Intervals (eV) in the effective absorption spectrum of PbS with different β - quantum outputs	0,3÷1,2 β ≤ 1	1,2÷1,8 β ≤ 2	1,8÷2,4 β ≤ 3	2,4÷3 β ≤ 4	>3
The share of light absorption energy (%)	11,8	14,7	24,0	19,2	30.3
The average value of the energy (eV) of the radiation quantum in the ranges	1,05	1,55	2,25	2,55	3.45
The number of effectively absorbed photons by the frontal part of the NHJ in PbS (photon/(s·m^2)-N^i_{PbS})	$0{,}63\cdot10^{21}a^2$	$1{,}07\cdot10^{21}a^2$	$1{,}8\cdot10^{21}\cdot a^2$	$1{,}69\cdot10^{21}\cdot a^2$	$2{,}75\cdot10^{21}a^2$
The fifth column shows the fraction of radiation ($\hbar\omega$ > 3 eV) that leads to heating of the solar cell ($2{,}75\cdot10^{21}\cdot a^2$)					

Having reached the contact field of the nanoheterojunction, the electron-hole pairs born in silicon N_{Si} are separated there. The sum of nanoheterojunctions and N_{Si} determines the number of effectively absorbed photons in the nanoheterojunctions <PbS:Si>:

$$N = N(a,b) = N_{PbS} + N_{Si} = 5{,}2\cdot10^{21}\cdot a^2\cdot[1 + (b^2/a^2)\cdot2{,}75/5{,}2\ ].$$

If $a^2/b^2 << 1$, then the absorption contribution to "a^2" will be small. It follows from the table that about 70% of the spectrum of incident solar radiation is effectively absorbed in PbS due to successive manifestations of the effects of multiplication of carriers and multiexciton generation. And although the absorption of solar radiation in PbS is relatively small (about a percent), but its contribution to the creation of a strong contact field in the nanoheterojunction is significant.

4. CONCLUSION

It follows from the above that efficient and promising photovoltaic systems can be created on the basis of non-crystalline silicon in combination with semiconductor nano crystals PbX. The question of using non-crystalline silicon as a substrate of an effective solar cell is considered. It is shown that this is possible only at high densities of localized defective energy states in the depth of the silicon band gap. In addition, a particularly effective conversion of solar energy into electricity is possible when two materials are combined as components of heterojunctions: non-crystalline silicon and lead chalcogenides in the nano-dimensional state, taking into account their specific optical and electrophysical properties.

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