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Simulation-based investigation of Depleted hetero-junction CdS/PbS (bulk and quantum dot) solar cell

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Abstract

The influences of conduction band position of PbS absorber on the performance of solar cells, including open circuit voltage, short circuit current density, fill factor and power conversion efficiency, has been simulated. It was obtained that for bulk PbS absorber layer the short circuit current density is higher than that of PbS QD, because there are a high density of surface traps in the band gap of PbS QD which leads to decrease in short circuit current density by creating series resistance.But the open circuit voltage in device containing of PbS QD is significantly higher than that of bulk PbS because of the passivation of electron- hole recombination process. The results of this simulation are significant in the utilize of PbS QD to optimize the hetero-junction solar cells.

Keywords: Depleted hetero-junction solar cells; Simulation; SILVACO; Surface trap.

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1. Introduction

Quantum dots (QD) or semiconductor particles are emerging as promising materials for optoelectronic devices such as solar cells, photo-catalysts, light emitting diodes, and photo-detectors. The most impressive aspect of Quantum dots (QDs) is their band gap which could be tuned by changing their size based on the quantum confinement effect. This property of QDs allows absorbing a relatively wide range of wavelengths from the visible to the near infrared, as well as plays fundamental role in electrical and optical properties.

Using of multiple semiconducting materials allows the absorbance of a wider range of light wavelengths, improving the cell's sunlight to electrical energy conversion efficiency.

Among various kinds of II–VI compound semiconductor nanoparticles, Cadmium Sulfide (CdS) is widely studied as its direct band-gap energy (of 2.4 eV) is located in the visible region which is suitable for photovoltaic devices [1-3].

Lead sulfide (PbS) is another quantum dot material which has attracted more attentions because of its considerably narrower bulk band gap of about 0.4 eV. Therefore it extends the absorption band to the near infrared region of the solar spectrum [4].

In our previous work [5] we used CdS quantum dot as light absorber material and simulated a CdS quantum dot sensitized solar cell (CdS QDSSC) using the Silvaco-Atlas software, which a power conversion efficiency of 1.8% was obtained.

Here we simulate a p-n junction solar cell composed of a p-type PbS QD layer on top of a n-type CdS QD layer. In this simulation, we benefit of Size-effect tuning ability of PbS QD which causes to obtain a depletion region for effective field-driven charge transport and separation separation at the CdS/PbS interface to get higher J_{SC}.

The aim of this work is to obtain the maximum power conversion efficiency of a p-n junction solar cell with FTO/CdS/PbS/MoO_3/Ag structure. The effect of the QD size on the electrical parameters of the solar cell was investigated.

2. Modeling and Simulation

In solar cell simulation, materials should be carefully chosen to maximize the light absorption (especially visible and infrared regions) to produce a high short circuit current density (Jsc), large open-circuit voltage (Voc), fill factor (FF), and finally the power conversion efficiency (η).

The conversion process of light energy into electricity requires a material to absorb photons. These absorbed photons raise electrons from ground states to higher energy ones, which leave holes in the valence band, and therefore, electron- hole pairs (excitons) are created. Separation of these electrons and holes is done by an electric force (caused by "built-in" electric field) existing at the p-n junction. Near the junction, electrons combine with holes and create a "depletion region". This junction moves electrons to the n-type side and holes to the p-type side of the junction. Generated excitons are converted to electrons and holes due to this separation and then flowed to an external circuit.

The resistance of the depletion region could be modified by applying an external electric field to the "built-in" electric field. If the external electric field is in the same direction as the "built-in" electric field, the depletion region's resistance will become greater. Otherwise, the depletion region's resistance will become smaller. Therefore, the depletion region could be considered to operate as a voltage-controlled resistor.

On the other hand, the work function (WF) of transparent conducting oxides (TCO) significantly impacts the performance of solar cells because the TCO WF affects the band alignment between TCO and absorber [6].

In inverted architecture, Indium doped Tin Oxide (ITO) or Fluorine doped Tin Oxide (FTO) forms the electron-collecting electrode (anode) and a high work function metal, such as silver forms the hole-collecting electrode (cathode).

3. Results and Discussion

3.1. Structure

A single junction solar cell with FTO/CdS/PbS/MoO_3/Ag structure is studied using two-dimensional numerical computer simulation software (ATLAS from Silvaco). Atlas is a module of SILVACO which predicts the electrical behavior of specified semiconductor structures [7].

All simulations were done under normalized conditions, a temperature of 300 K, and AM1.5 illumination. The structure of the p-n junction solar cell consists of a P-type PbS and N-type CdS along with energy level diagrams for

devices consist of PbS bulk and PbS QDs (with QD diameter of ~ 7 nm) are shown in figure 1.

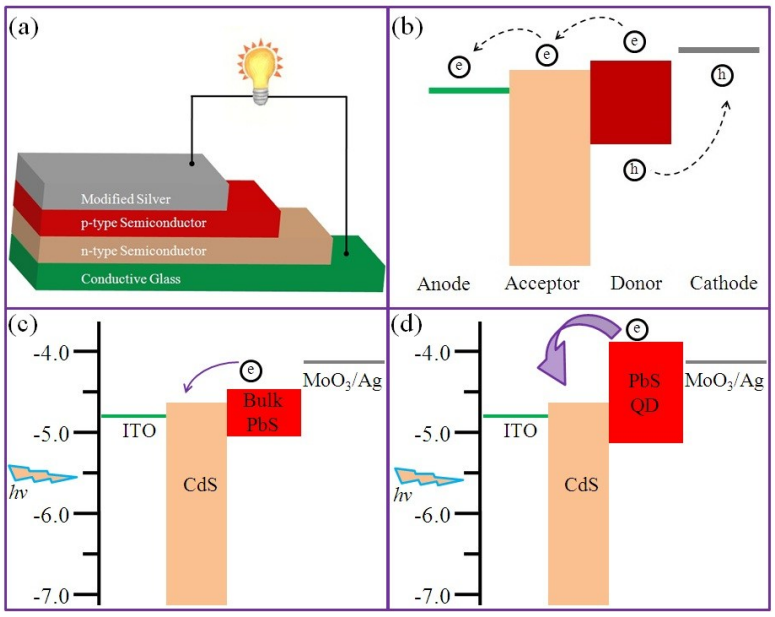

Figure 1 Scheme of depleted hetero-junction device

The band gap and electron affinity level (EA) of bulk PbS are about 0.41 eV and 4.6 eV, while these parameters for bulk CdS are 2.4 eV and 4.7 eV, respectively.

Figure 2 shows scanning electron microscopy (SEM) image of the fabricated PbS QD along with its band gap energy calculated by Tauc formula [8].

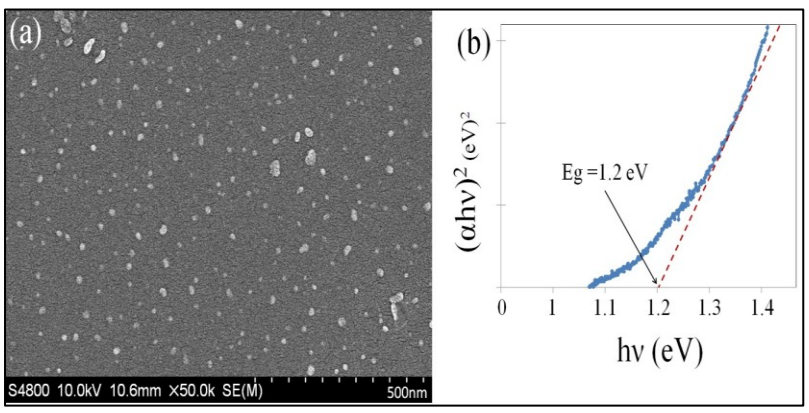

Figure 2 (a) SEM image of PbS QDs on glass substrate, (b) the energy gap of PbS QDs

As shown in figure 1, the solar cell is illuminated from ITO side, and electrons and holes are created in active layer (PbS). These electron- hole pairs should move toward contacts to create electric current. In such situation which the difference between C.B of CdS and PbS is about 0.1 eV, electrons couldn't transfer effectively.

Quantum confinement effect in PbS nanocrystals could increase the optical band gap up to ~1.5 eV, shifting the EA above the C.B level of CdS [9, 10].

According to Marcus theory, electron transfer rate from conduction band (C.B) of PbS (donor) to the C.B of CdS (acceptor) increases with increasing the energy difference of C.B of donor and acceptor (figure 1 (d)).

In our p-n junction structure, surface recombination and Shockley-Hall-Read recombination processes should be considered, which is introduced by SURF.REC and SRH model in the model statement, respectively. Figure 3 shows the J-V curve of our device in the architecture ITO/CdS/PbS /MoO_3-Ag with two kinds of absorbers.

This curve could be expressed by the generalized Shockley equation

$$I = I_{pv} - I_0\left[\exp\left(\frac{q(V+IR_s)}{n_D k_B T}\right) - 1\right] - \frac{V+IR_s}{R_{sh}} - r_{Rec.}I_{pv}$$

Where I_{pv}, I_0, n_D, R_s, R_{sh}, k_B and T are photocurrent (which delivered by the constant current source), reverse saturation current (corresponding to the diode), ideality factor (which takes into account the deviation of the diodes from the Shockley diffusion theory), Series Resistance (which takes into account losses in cell solder bonds), shunt resistor (which takes into account the current leakage through the high conductivity shunts across the p-n junction) Boltzmann constant, and the absolute temperature of the p–n junction, respectively [11]

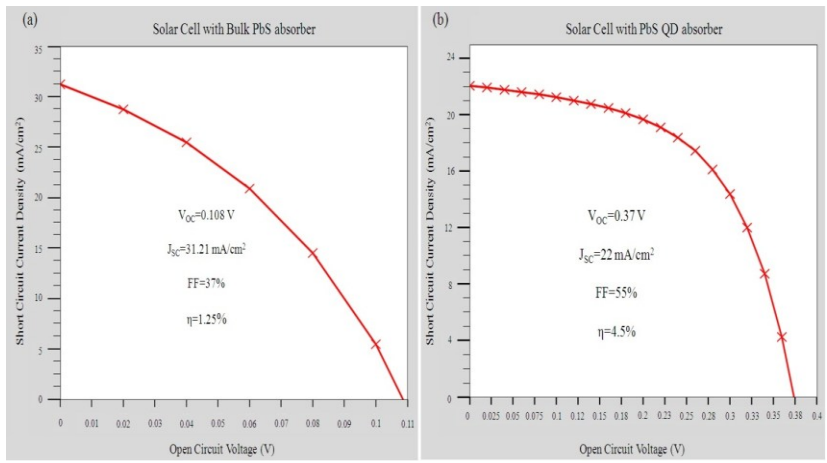

Figure 3 The J-V curve of device with (a) Bulk PbS, (b) PbS QD absorber.

Two kind of PbS layer as absorber materials have been tested on CdS. Table 1 summarizes solar cell parameters obtained in present work.

Table 1 Photovoltaic properties of devices containing of bulk PbS and PbS QD

Absorber	J_{SC} (mA/cm^2)	V_{OC} (V)	FF(%)	η (%)
Bulk PbS	31.21	0.108	37	1.25
PbS QD	22	0.37	55	4.5

In the device containing of bulk PbS with the band gap of 0.41 eV, a short circuit current density (J_{SC}) of 31.24 mA/ cm^2 was reached but the fill factor (FF) was only about 0.37. The band gap of PbS has been increased up to 1.2 eV by decreasing the particle size. A significant decrease in J_{SC} with the decrease in average diameter of PbS nano-particles was demonstrated, which is a strong indication of the quantum confinement effect [12].

The strong reduction of JSC (from 31.21 mA/cm^2 to 22 mA/cm^2) is caused by decreasing the light absorption with increasing the band gap.

From Table 1, it could be observed that the open circuit voltage (V_{OC}) is increased by using PbS QDs as absorber layer which caused by reduce in band to band recombination process in the PbS, as shown in figure 1(d). This reduction in recombination is mainly caused by an improved in local separation of charge carriers and their transport to the external loads.

3.2 Forces Acting on Electrons and Holes

In the p-n junction, the n-type layer spare electrons jump over to fill the gaps in the p-type material. Therefore, n-type material becomes positively charged, and the p-type material is negatively charged. The small volume in which this space charge is created is called depletion layer which there is a strong electric field (E) in this area. Photo-generated electrons and holes are exposed to this electric force (E).

The electric field in depletion region of CdS/bulk PbS and CdS/PbS QD interfaces are shown in figure 4 (a, b), respectively.

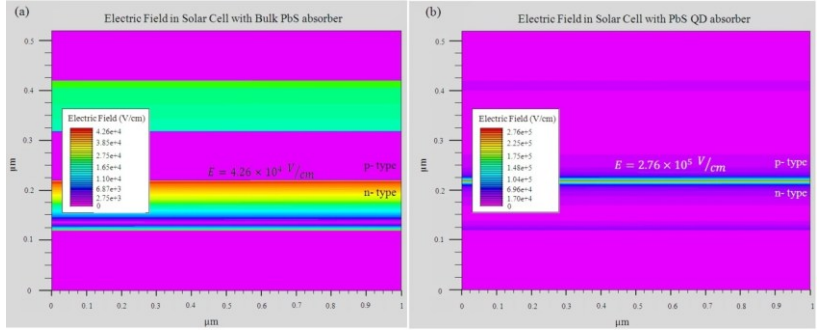

Figure 4 Electric field in solar celwith (a) Bulk PbS, (b) PbS QD.

In this case, the charge current of electrons (and holes) with a charge of q (=Ze) and a concentration of n is given by [13]

$$\vec{J} = ne\mu\vec{E} = \overrightarrow{\sigma E} = -\frac{\sigma}{q}\vec{\nabla}(q\varphi)$$

Where μ, σ, qφ are the mobility, electrical conductivity, and the electric force acting on the electrons (and holes), respectively.

The potential across the depletion region in thermal equilibrium is called built in potential (V_{bi}) and equals to the voltage drop through the p-n junction.

V_{bi} is equal the difference between the fermi energies of each region, which is shown in figure 5.

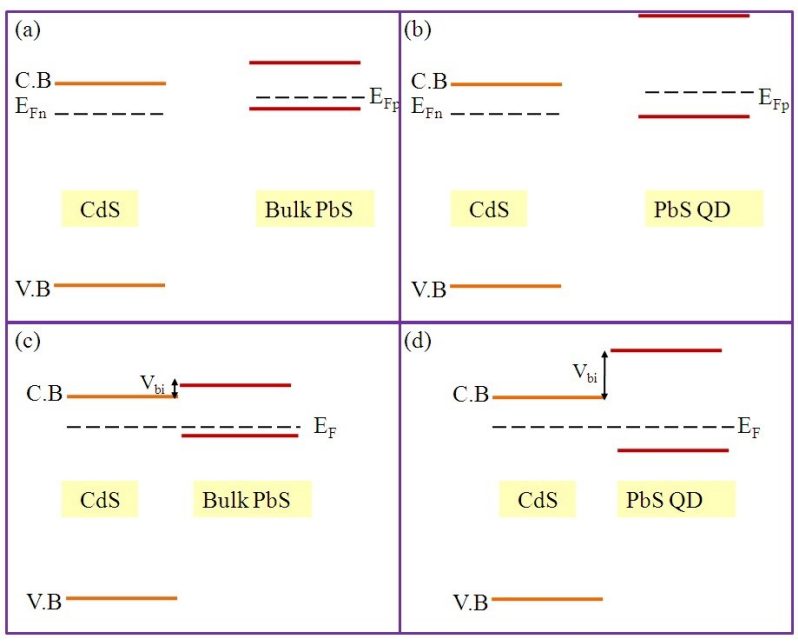

Figure 5 Band diagrams of (a, b) n-type and p-type semiconductors before contact, (c, d) Fermi level alignment and built in potential across the depletion region of p-n junction

The built in potential (V_{bi}) is calculated by following equation:

$$qV_{bi} = E_g - E_{Fn} - E_{Fp}$$

Where E_{Fn}, E_{Fp} are the values of the Fermi levels of the n-type and p-type semiconductors, respectively.

Further, figure 4 reveals a higher V_{bi} in case of PbS QD compared to bulk PbS suggesting the presence of high density of surface traps within the band gap of PbS QD and is expected to be due to increased surface to volume ratio with decreasing the crystalline size of PbS. As existence of surface traps creates series resistance (R_s), the short circuit current density has been decreased from 31.21 mA/cm^2 to 22 mA/cm^{2}for bulk PbS and PbS QD, respectively.

We calculated the depletion width of both CdS/PbS junctions (bulk PbS and PbS QD) which was found to be 2.38 μm and 1.30 μm, respectively.

The various parameters of both bulk PbS and PbS QD are summarized and given in Table 2.

Table 2 Different parameters of bulk PbS and PbS QD

Parameter	Value for Bulk PbS	Value for PbS QD
Band gap (E_g)	0.41 eV	1.2 eV
Barrier height (qV_{bi})	0.1 eV	0.35 eV
Electron affinity (χ)	4.6 eV	3.9 eV
Depletion Width (W)	2.38 μm	1.30 μm
Conduction band edge (C.B)	4.6 eV	3.9 eV
Valence band edge (V.B)	5.01 eV	5.1 eV

6. Conclusions

We have simulated and obtained the photovoltaic properties of both CdS/bulk PbS and CdS/PbS QD hetero-junctions. Interestingly, it was found that a high density of surface traps is created within the band gap of PbS QD which creates series resistance and decreases the short circuit current density. However, using of PbS QD leads to increase the band gap of PbS which increases the open circuit voltage by reducing the electron- hole recombination rate.

Therefore, using the PbS QD absorber instead of bulk PbS has 2 opposite effects on the cell performance. Negative effect tends to decrease the J_{SC} but the positive effect refers to increase the V_{OC} by reducing the recombination rate. As a result, by choosing a suitable particle size, higher power conversion efficiency could be obtained.

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