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ORIGINAL ARTICLE

Introducing nanostructure patterns for performance enhancement in PbS colloidal quantum dot solar cells

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Abstract

With attention to the thin film structure of colloidal quantum dot solar cells, in this paper in order to improvement of active layer absorption of them, we have proposed the use of nanostructure pattern for enhancement of their performance. For this purpose we have presented suitable nano hemisphare patterns in colloidal quantum dot solar cells for light trapping in absorption layer. Then with simulation of the obtained nanostructure solar cells we have studied on improving the absorption spectrum and thus increasing the short circuit current density of them. In order to simulation of light propagation in nanostructures, we have used finite-difference time-domain method. According to the calculation results and with optimization of periodic nanostructure patterns, we have shown that short circuit current density has been increased up to 15.95%. Absorption spectrum, quantum efficiency density and short circuit current density have been discussed for colloidal quantum dot solar cells nanostructures with low and high thickness of absorption layer in this paper.

Keywords: *Colloidal Quantum Dot; Finite Difference Time Domain; Nanostructure Pattern; Quantum Efficiency; Thin Film.*

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INTRODUCTION

With population growth the rate of energy consumption will be so high and this will be serious risk for fossil fuels in near future. Since, for answering human need we must have clean fuel without need to fossil fuels. For this purpose solar power is cleaner and cheaper source of the energy [1]. Photovoltaic converts directly sunlight into electricity by small panels of semiconductors, which is called solar cell [2]. Recent agreement of Paris determines an aim for limiting CO_2 publication in atmospheric and limiting temperature increase that any country must attempt for doing something in solving these problems. Sun energy is as a plentiful, attractive and hopeful source for decreasing and also replacing of fossil fuels [3]. Solar cells on basis of crystal silicon have been commercialized widely until today. However according to the limits of these types of solar cells, researchers are searching for suitable replacements that have lower production cost and higher power conversion efficiency. Solar cells on based of colloid quantum dots are one of the hopeful nanostructure cells. In recent years, this type of solar cells has been researched widely. Colloid quantum dots (CQD) solar cells are suitable replacement for silicon solar cells because of their unique properties [4-7]. PbS colloidal quantum dot solar cells have attracted great interest for tunable absorption spectrum of them with quantum dots size [8-10] and low cost potential of them due to their facile processable features [11-14]. CQD solar cells have different types that can be classify as main topics that have been discussed in: quantum dot Schottky junction solar cells [15], quantum dot solar cells with inhomogeneous junction,

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quantum dot solar cells with thin absorption layer [16] and quantum dot-sensitized solar cells [17]. In 2010, researchers proposed a successful constriction for inhomogeneous junction solar cells with colloidal quantum dot that eliminate main limitation of schottky junction solar cells (low internal voltage) [13]. The advantage of inhomogeneous junction solar cell to schottky junction solar cells is that in schottky type, light incidence to junction from quantum nanoparticles, so electrons and holes form in a place far from junction. While in inhomogeneous junction, light enters from n type semiconductor material with high band gap, so this layer dose not absorb light and much density of electrons and holes product in quantum dot layer near to junction place thus absorption occurs in an effective way. There are two essential methods for absorption improvement and thus performance enhancement of thin film solar cells: 1) Replacing flat layer structures with nano pattern layer structures 2) Using of materials that have better absorption such as PbS for absorption layer. Nano science that has been discussed in this paper is related to photovoltaic phenomena and plays an important role in directly generation of electrical energy from solar energy. Nano structure patterns that have been known as different forms such as spherical, cubic, wire, tube, ribbon, ring and in the form of plate that have important role in light beams absorption of thin film solar cells [18-23]. In this paper we have used nanostructure patterns of periodic hemisphere that have created from colloid quantum dot PbS as absorption layer and other back layers have formed according to it. In order to introduction of optimal nanostructure of colloid quantum dot solar cells we have investigated effect of period of nanostructure in different thickness of absorption layer (PbS layer). Then we have selected the best structure of them that has the best improvement for quantum efficiency and short circuit current density (J_{sc}).

We have applied FDTD method for stimulation of light propagation and solving Maxwell's equations. To achieve these purposes in first part we have studied on simulation method and proposed structure material. In second part we have introduced optical analyzing of flat structures and periodic hemispherical nanostructures of CQD solar cells. Finely in third part we have discussed about the results and proposed the best nanostructure for colloid quantum dot solar cells.

MATERIALS AND METHODS

SIMULATION METHOD

In this paper we have used of finite difference time domain method (FDTD) solution software for investigating publication of light waves in colloid quantum dot solar cells. All of the simulations have been done in 2D model [24-26]. In FDTD method with solving Maxwell equations, electrical (E) and magnetic (H) fields that have been continuous functions at first, have been returned to discrete functions. Thus fields as a function of time (nΔt that briefly shown as n) have been obtained by discrete-time state equation of (1) and (2).

$$\vec{E}^{(n+1)} = \vec{E}^{n} + \frac{\Delta t}{\varepsilon}\vec{\nabla} * \vec{H}^{(n+\frac{1}{2})} \quad (1)$$

$$\vec{H}^{\left(n+\frac{3}{2}\right)} = \vec{H}^{(n+\frac{1}{2})} - \frac{\Delta t}{\mu}\vec{\nabla} * \vec{E}^{(n+1)} \quad (2)$$

By obtaining the distribution of field from (1) and (2) equations, we have been used the equation (3) to extract quantum efficiency.

$$QE(\lambda) = \frac{1}{p_{\text{opt}}}\int \frac{1}{2} c\varepsilon_0 n\alpha . \left|E(x,y,z)\right|^2 dxdydz \quad (3)$$

Where c is the speed of light in free space, is vacuum permittivity coefficient, a is energy absorbing coefficient (a= 4πk/), n and k are real and imaginary parts of refractive index, λ is wave Length, E is electrical field and P_{opt} is the power of incidence light. For computation short circuit current density (J_{sc}) we have used (4).

$$J_{sc} = \frac{q}{hc}\int_{\lambda_{\min}}^{\lambda_{Max}} \lambda . Q\, E(\lambda)\, S(\lambda)\, d\lambda \quad (4)$$

That q is elementary charge of electron, h is plank constant, S(λ) is spectrum of sun light (solar irradiance spectrum AM 1.5G).

Proposed flat structure materials

In this paper, we have used of flat structure according to Fig. 1 for first simulation. Our flat structure have been formed from glass layers as substrate, ITO as transparent conductor layer, TiO_2 as electron carrier layer, PbS as absorption layer and Au as metal contact. Flat structure layers with primitive thickness have been shown in Fig. 1(a). Optical constants (n, k) of each layer in the device have been taken from previous literature [27], that have been determined by ellipsometric measurements in T=300 k operating temperature, and have been used as input parameters in our optical simulation model. Also the formation of

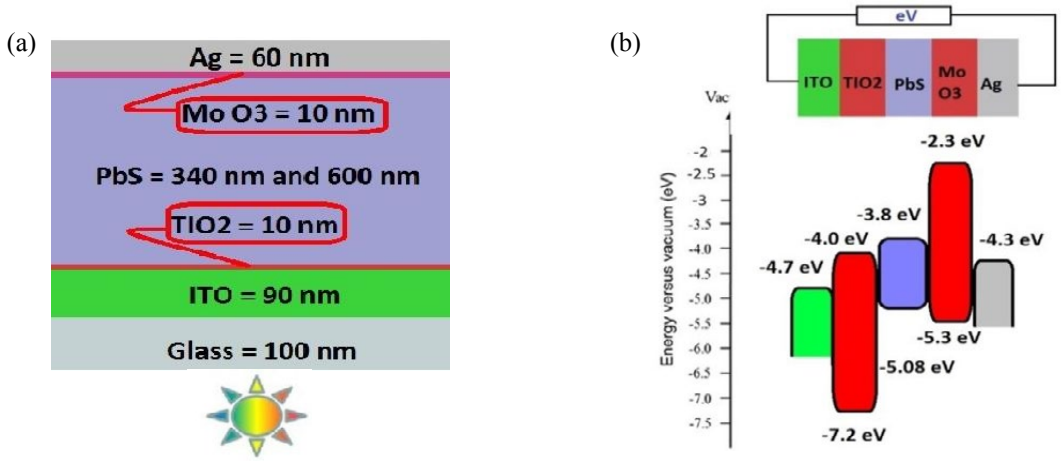

Fig. 1. (a) Simulated view of flat structure layers of CQD solar cell and (b) Energy band diagram for different layers of colloid quantum dot solar cell.

energy band diagram for different layers that lead to configuration suitable photo current in solar cell structure, have been shown in Fig. 1(b).

RESULT AND DISCUSSION

Optical analyzing of flat structure CQD solar cell

First we have designed and stimulated our flat structures. In our simulation we have calculated absorption spectrum, general short circuit current and quantum efficiency for each structure. Since the absorbing layer plays the most effective role in improving the photo current, absorption spectrum calculations have been considered for the PbS absorber layer. Flat structures with PbS absorber layer have been simulated in two low and high thickness (340nm and 600nm). The calculated absorption spectrum for flat structure with low and high thickness of absorber layers are compared in Fig. 2. The results are in good agreement with the calculated results in [27] (as 340nm and 600nm are optimized thicknesses that have been obtained in this reference we have chosen these thicknesses for study in our structures), which have indicated the accuracy of the calculations that have been performed in this paper. According to the results of Fig. 2, the absorption spectrum in a 600 nm state is better than the 340 nm ones, and it can be seen by comparing and calculating the total short-circuit current for two structures. The short circuit current density (J_{sc}) obtained for this structure have been compared in Table 1. The results show that in the flat structure states, the change in thickness in the absorption layer from 340 nm to 600 nm resulted in an increase of 20.35% of the total current. But since the carrier diffusion length is limited, obtaining suitable absorption for absorber layer in low-thickness conditions is much more desirable.

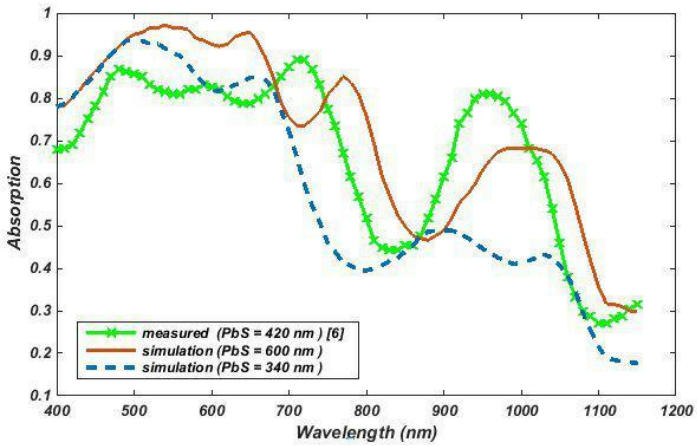

Fig. 2. The absorption spectrum of flat structures with two different thicknesses of absorbent layer.

Table 1. Total current of absorber layer.

Type of Material	Thickness	J_{sc}
PbS	340 nm	26.58 mA/cm^2
PbS	600 nm	31.99 mA/cm^2

On the other hand with computation of generation rate for different layers in flat structure with low thickness of absorber layer (340nm) we have seen that much generation rate have been created in PbS layer and in this layer the much scope for generation rete have been related to bottom level (Fig. 3). Thus we have tried to increase the generation rate in the other levels of absorber layer too. Need to explain that the generation rates in the other layers are parasitic effects thus there is not any effective absorption in these layers that leads to photocurrent.

Optical analyzing of periodic hemisphere pattern Nano structure CQD solar cell

In this section in order to improvement of absorption spectrum and as a result increment of total sort circuit current we have replaced flat structure with nanostructure pattern CQD solar cells. Our introduced structure have been constructed from nanostructure patterns of periodic hemisphere that have created from colloid quantum dot PbS as absorption layer and other back layers have formed according to it on flat substrate of TiO_2 (Fig. 4(a)). We have simulated this structure with different thickness and different periodic constant and introduced the optimal structure with best results. For these purposes the wave lengths of stimulation have been regulated from 400 nm to 1100 nm. In continue, with calculated results, generation rate has been

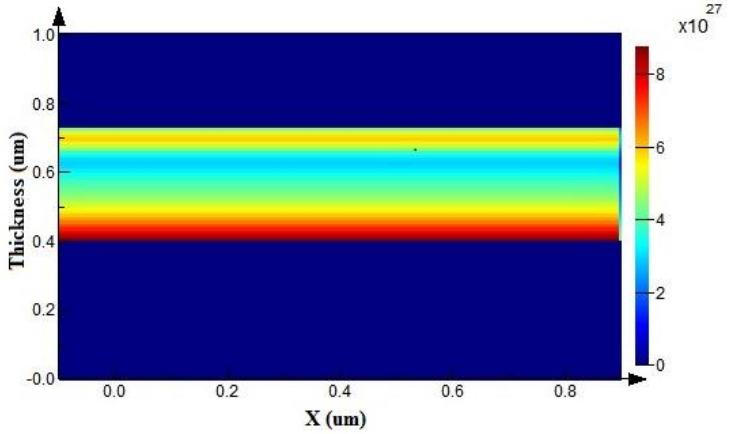

Fig. 3. Generation rate for sun light beaming in flat structure CQD solar cell with low thickness of absorber layer (PbS=340 nm).

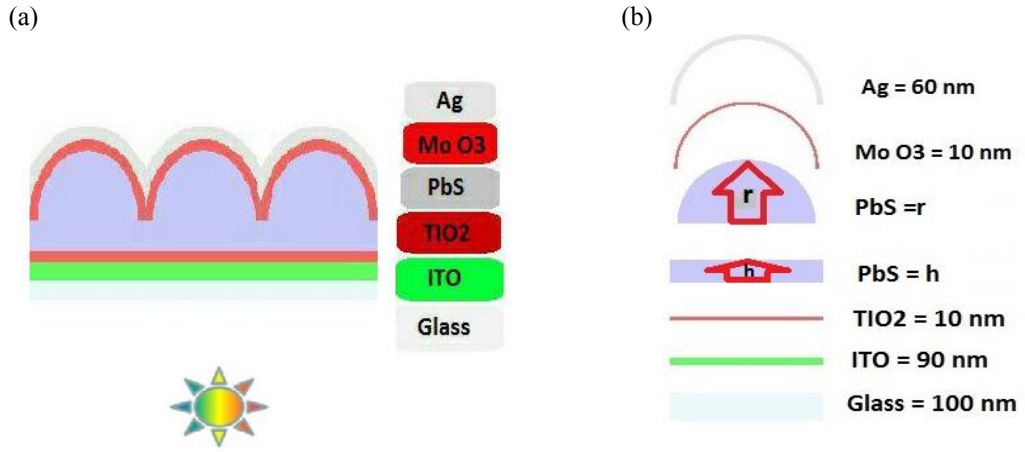

Fig. 4. (a). Simulated view of nanostructure pattern layers of CQD solar cell and (b) Specifications of layers for hemisphere nanostructure pattern.

obtained for different layers of CQD solar cell in standard solar spectrum of AM1.5G. In Fig. 4(b) complete properties of structure layer thickness and radius of hemisphere have been shown. We take layer thickness of PbS in two flat layer with h thickness and hemisphere pattern with r radius. The structures have been stimulated with different amount of r and h and the results have been compared for obtaining optimum results.

In Fig. 5 we have shown whole view of nanostructure CQD solar cell with 2D hemisphere pattern in software simulation environment. The results that have been obtained from calculated absorption spectrum for nanostructure CQD solar cell with low thickness absorber layer in 4 state (A: h=140 nm, r= 400 nm, B: h=190 nm, r = 300 nm, C: h= 240 nm, r=200 nm, D: h = 290 nm, r=100 nm) have been compared in Fig. 6. Then The results that have been obtained from calculated absorption spectrum for nanostructure CQD solar cell with high thickness absorber layer in 4 state (E: h=250 nm, r=700 nm, F: h=350 nm, r=500 nm, G: h=450 nm, r=300 nm, H: h=550 nm, r=100nm) have been compared in Fig. 7. The states have been selected such that the sum of h and average of r for the low thickness state has been equal to 340 nm (r/2+h=340nm) and for the high thickness it has been equal to 600 nm (r/2+h=600nm). With comparing the absorption spectrum in wave length range between 400 nm and 1100nm for different states in low and high thickness as shown in Fig. 6 and Fig. 7, respectively B and G states have obtained the highest absorption spectrum.

We have calculated short circuit current for all of the states and compared the results in Table 2 and Table 3. We have obtained from the results that the highest short circuit current in low thickness condition creates for B state that have increased 15.95% rather than flat structure. This means that with preserving carrier diffusion length in 340 nm

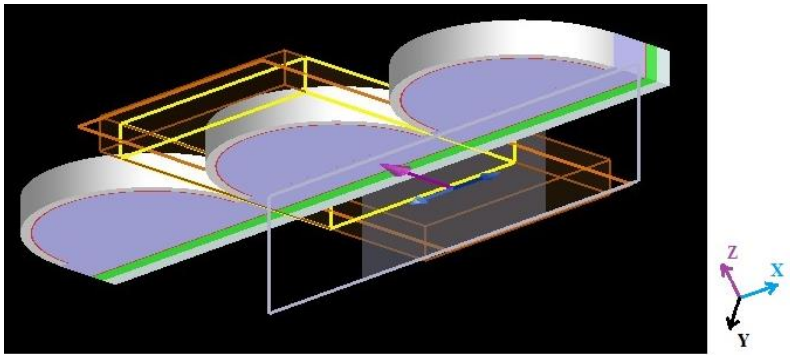

Fig. 5. Whole view of hemisphere nanostructure pattern in stimulated environment.

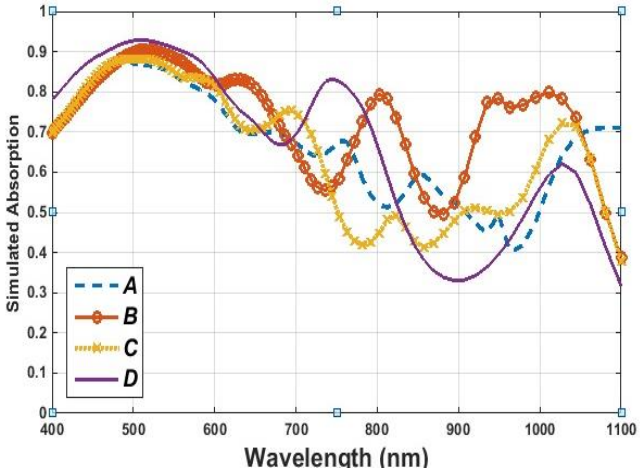

Fig. 6. Absorption spectrum of nanostructure CQD solar cell absorber layer with low thickness in 4 states A, B, C and D.

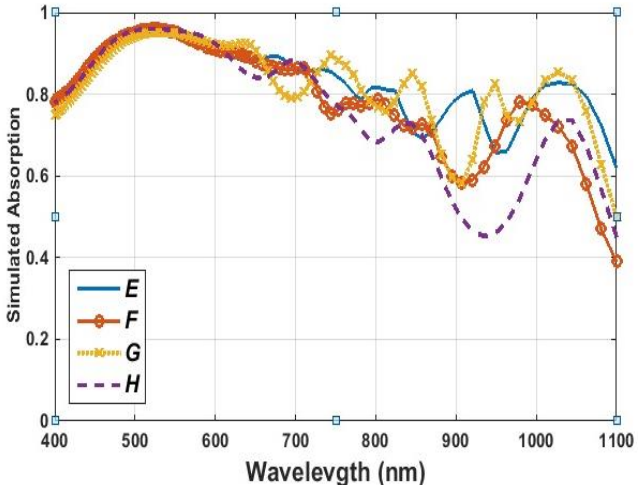

Fig. 7. Absorption spectrum of nanostructure CQD solar cell absorber layer with high thickness in 4 states E, F, G and H.

Table 2. Total current of absorber layer for nanostructure solar cell with low thickness in 4 states.

states	Thickness	J_{sc}
A	h=140nm, r=400nm	28.40 mA/cm^2
B	h=190nm, r=300nm	30.82 mA/cm^2
C	h=240nm, r=200nm	27.67 mA/cm^2
D	h=290nm, r=100nm	28.66 mA/cm^2

Table 3. Total current of absorber layer for nanostructure solar cell with high thickness in 4 states.

States	Thickness	J_{sc}
E	h=250 nm, r=700nm	33.37 mA/cm^2
F	h=350 nm, r=500nm	33.67 mA/cm^2
G	h=450 nm, r=300nm	35.79 mA/cm^2
H	h=550 nm, r=100nm	32.69 mA/cm^2

we have improved short circuit current and thus enhanced performance of CQD solar cells. Also according to high thickness condition results the highest short circuit current have been obtained for G state that have been increased 11.8% rather than flat structure. With considering these descriptions as the power conversion efficiency (η) of solar cells that is equal to (where FF represents fill factor, V_{oc} denotes open circuit voltage, J_{sc} is the short circuit current and P_0 is input power) will be improved with photo current enhancement. With computation of generation rate for active layer of CQD solar cell in B state nanostructure pattern as we have shown in Fig. 8, the generation rate has been spread in whole levels of absorber layer and

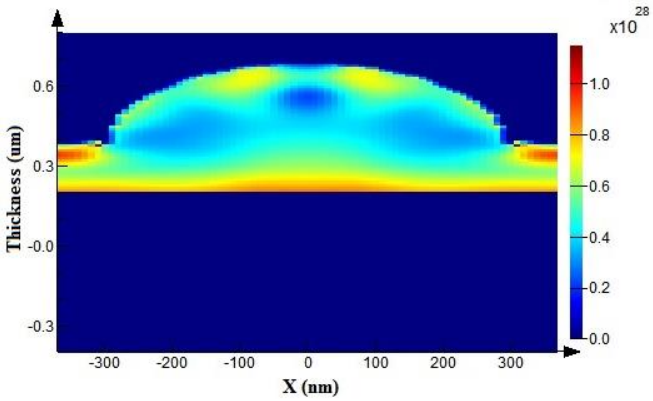

Fig. 8. Generation rate for sun light beaming in B state nanostructure pattern CQD solar cell.

this has been lead to improvement in absorption spectrum and thus increasing short circuit current rather than flat structures.

CONCLUTION

In this paper, we have improved absorption spectrum and thus increased the short circuit current of CQD solar cells with the use of hemisphere nanostructure pattern. Then with consideration of the free carrier diffusion length limit, we have optimized our presented nanostructure for CQD solar cells. This increases of short circuit current for structures with low thickness is from 26.58 mA /cm^2 in flat structure to 30.82 mA /cm^2 in nanostructure pattern CQD solar cell with B state (B: h=190 nm , r=300 nm). This structure with serving electrical thickness equal to flat structure, have been shown 15.95% increase in short circuit current. Also this increases of short circuit current for structure with high thickness is from 31.99 mA /cm^2 in flat condition to 35.79 mA /cm^2 in nanostructure pattern CQD solar cell with G state (G: h = 450 nm , r= 300nm). In this condition we have obtained 11.8% increase in short circuit current rather than flat structure with preserving of electrical equal thickness. Thus in whole, CQD solar cells on basis of PbS with nanostructure patterns have been shown better absorption spectrum so have been produced better current density than flat structures. The reasons for these improvements have been obtained for optical effective thickness increment, that have been created with adjusting the solar cell structure architecture and thus with improving in light trapping more than before in absorber layer.

DISCLOSURE STATEMENT

All authors declare that they have no conflict of interest in the publication of this manuscript.

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