

Effect of Absorption Coefficients in Upper Efficiency Limit of Intermediate Band Solar Cells

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ABSTRACT:

In this paper, the idea of an intermediate band solar cell which increases the efficiency of solar cells is considered. By using quantum dots the idea of intermediate band solar cell can be achieved at an acceptable level. Actual results of using quantum dots have led to decreased efficiency of solar cells. The effect of absorption coefficients on the upper limit of efficiency in special types of solar cells is the focus of this paper. The main factors that have the most impact on the upper limit of efficiency of our position of intermediate bands and consequently the structure of quantum dots are analyzed. Furthermore, the changes in cell characteristics, quantum dot type, quantum dot structure, and even polarization of the incident light can change the upper limit of efficiency. Changes in distance layers of quantum dots create different results for different polarization of light for the upper limit of efficiency. Using the results of this research can be a way to new research in the field of solar cells with quantum dots and the optimum use of solar cells will be useful.

KEYWORDS: Band Position, Detailed Balance Theory, Output Power Reduction, IBSC.

1. INTRODUCTION

One of the most important methods for increasing the efficiency of solar cells is the application of the intermediate bands because of increasing of output current by absorption of photons with energies below the band gap. By using this technique, the upper limit of efficiency, based on detailed balance theory, is increased from about 40% [1] for the solar cell without an intermediate band to about 60% with one intermediate band [2]. This significant rise has attracted the attention of many researchers. One of the major challenges of this research is the realization of the intermediate band. Some ways to create intermediate band gap energy of the semiconductor solar cell substrate include creating special doping with appropriate energy balance [3-5], quantum wells [6-8], quantum dots [9-12], and highly mismatching alloys [13-15]. However, the creation of energy levels due to the special doping with appropriate energy balance because of low level of concentration does not have the characteristics of a band and despite allowing the absorption of low energy photons does not guarantee a dramatic increase in performance. Using quantum dots is preferable to quantum wells because, in addition to the isotropic nature of the incoming light, the quantization of energy levels in quantum dots is in three dimensions while in quantum wells is in one dimension. Highly mismatched alloys, with convenient features that make the intermediate band, their presence does not cause a dramatic increase in performance. As a result, it appears that the proposed methods achieve an intermediate band using quantum dots that can be a further increase in performance. In the first research, (for example [16]) actual results of using quantum dots were against the expected results because these changes caused to decrease the solar cell efficiency. This reduction is contrary to the goals of the researchers then they decided to examine the reasons for this occurrence. Along with this research, attention was paid to the absorption of photons in these structures, because in addition to solar cells [17-18], have a main effect on the photo-detectors [19-20]. Luque et al proposed a model for the transfer of the central bands of bound states in a solar cell

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for calculating the absorption coefficient [21]. Luque with regard to the transition between the intermediate band and conduction band completed the previous research [22].

The structure of this paper is as follows. In sections 2 and 3, the absorption coefficient calculation method and the upper efficiency limit of this type of solar cell are explained. At the end, the results of our work are presented.

2. THEORETICAL BACKGROUND

The relationship between photon absorption coefficients in an absorbing layer containing quantum dots is as follows [23]:

$$\alpha(E) = \frac{2\pi^2 e^2 E}{n_{ref} c \epsilon_0} \times \frac{|\langle \psi | r \cdot \epsilon | \psi' \rangle|^2}{S} \times F N_l \delta(E - E_{line}) \quad (1)$$

Where E is the photon energy, ϵ is the light polarization vector, n_{ref} is the refractive index of the medium, F is the fractional coverage of the surface with QDs, N_l is the number of QD layers per unit length, S is the Effective cross-sectional area of each quantum dot, and E_{line} is the energy difference between the two states. It should be noted that the density of quantum dots is equal to $F N_l / S$ [23]. δ represents the effect of the statistical distribution dimensions of the quantum dots that is variable and is expressed as a Gaussian [22]:

$$\delta(E - E_{line}) \cong \frac{1}{\sigma\sqrt{\pi}} \exp\left(-\frac{(E-E_{line})^2}{\sigma^2}\right) \quad (2)$$

Where, σ represents the energy dispersion. This dispersion depends on the regularity of the sample, although the integrated values are independent of s . The energy dispersion has been set to 0.025 eV. In addition, $|\langle \psi | \epsilon \cdot r | \psi' \rangle|^2$ expression in equation (1) is called a square matrix element and ψ and ψ' , respectively, are the normalized wave functions of the first and last state.

The pin solar cell structure in this study is the structure of quantum dots on the i region. To calculate the absorption coefficient of the i -only cells containing quantum dots have been satisfied. The i -type GaAs semiconductor material and quantum dots made of In $_{1-x}$ Ga $_x$ As are assumed. The number and location of the intermediate bands in addition to the size of the quantum dots and the distance between them, by changing the mole fraction x can be changed.

For ease of calculation, the cubic model for quantum dots inside the region of i will be considered. Similar to the method presented in [22], the solution of the Schrödinger equation in quantum wells in three dimensions of the cube and the emergence of wave functions and continuity of the first derivative of the border, inside and outside the energy levels and wave functions of quantum dots are calculated.

To evaluate the effect of polarization in the calculation of absorption coefficients and ultimately upper limit of the efficiency, five different modes of light polarization are considered.

Assuming that the cells are in the z -direction, these five polarization states of light are:

- 1- Z Unpolarized Beam: In this case, the light emitted in the direction z and the light polarization vector that is perpendicular to the light beam can have any direction in the xy plane.
- 2- Y-Polarized Z-Beam: The light emitted in the direction of z and y is a vector in the direction of polarization of light.
- 3- X Unpolarized Beam: The light emitted in the direction of x and light polarization vector can have any direction in the yz plane.
- 4- Y-Polarized X-Beam: The light emitted in the direction of x and y is a vector in the direction of polarization of light.
- 5- Z-Polarized X-Beam: The light emitted in the direction of x and z is a vector in the direction of polarization of light.

To establish the effect of light polarization with respect to the Euler angles (φ, θ) we have defined:

$$r = xi + yj + zk \quad (3)$$

$$\epsilon = (\cos \varphi \sin \theta)i + (\sin \varphi \sin \theta)j + (\cos \theta)k \quad (4)$$

Therefore:

$$\begin{aligned} |\langle \psi | \epsilon \cdot r | \psi' \rangle|^2 &= \cos^2 \varphi \sin^2 \theta |\langle \psi | x | \psi' \rangle|^2 \\ + \sin^2 \varphi \sin^2 \theta |\langle \psi | y | \psi' \rangle|^2 &+ \cos^2 \theta |\langle \psi | z | \psi' \rangle|^2 \end{aligned} \quad (5)$$

According to [22], we can see that a necessary condition for the transition between two energy levels of quantum numbers is only the change of one direction x, y, or z, and other quantum numbers are unchanged. Also, due to the resulting wave functions are simply shown:

$$D_t = |\langle \psi | t | \psi' \rangle| = \int_{-l}^l \psi_t^* t \psi_t' dt =$$

$$A_n B_m \left(\frac{1}{(k_m + k_n)^2} \sin(l(k_m + k_n)) - \frac{l}{k_m + k_n} \cos(l(k_m + k_n)) \right) +$$

$$A_n B_m \left(\frac{1}{(k_m - k_n)^2} \sin(l(k_m - k_n)) - \frac{l}{k_m - k_n} \cos(l(k_m - k_n)) \right) \quad (6)$$

Thus we have:

$$|\langle \psi | \varepsilon \cdot r | \psi' \rangle|^2 = \cos^2 \varphi \sin^2 \theta \times D_x^2 +$$

$$\sin^2 \varphi \sin^2 \theta \times D_y^2 + \cos^2 \theta \times D_z^2 \quad (7)$$

Radiated photon polarization can be different and the latter is obtained by averaging the results. Square matrix element can thus be written as follows:

$$|\langle \psi | \varepsilon \cdot r | \psi' \rangle|^2 = \cos^2 \varphi \sin^2 \theta |\langle \psi | x | \psi' \rangle|^2 +$$

$$\sin^2 \varphi \sin^2 \theta |\langle \psi | y | \psi' \rangle|^2 + \cos^2 \theta |\langle \psi | z | \psi' \rangle|^2$$

$$= A |\langle \psi | x | \psi' \rangle|^2 + B |\langle \psi | y | \psi' \rangle|^2 + C |\langle \psi | z | \psi' \rangle|^2 \quad (8)$$

For all authorized transactions and considering the quantum numbers of each of the energy levels, the coefficients of the matrix elements for the above five types of polarization are shown in Table 1. As can be seen in terms of what quantum number has changed, the coefficients of these 5 modes of polarization are obtained based on the above table. Also, a necessary condition for the transition between the two bands is the change of x or y or z quantum numbers, and transfer to a band is allowed so that the parity of its quantum number is different with respect to the parity of the source band. Thus, as seen in the following table, if the parity of the source band is odd the parity of the destination band is even and vice versa.

The fullness of the intermediate band is effective in the evaluation of the absorption coefficient, so the two modes as [22] have been considered:

In the first case with the FF = 1 in the charts, the lowest intermediate band is half-filled, and other bands are assumed to be empty.

In the latter case with the FF = 2 in the charts, the lowest intermediate band is completely filled and the first excited energy levels are assumed to be half full and others empty.

Using the absorption coefficient obtained, we can obtain the probability of absorption. Absorption probability is equal to the product of the absorption coefficient on the distance traveled by light in the cell. By considering the size of the cell and the path traveled by light photons inside the cell, we can specify the length of the path traveled by the photon, and with it, the probability of photon absorption can be achieved.

3. CALCULATION METHOD

To calculate the upper limit of efficiency based on detailed balance theory and according to [24], the model of Fig. 1 for a cell with three intermediate bands is considered. Obviously, it will be extended to more or less the intermediate band.

In this circuit model, two circuit elements can be seen: the diode and the current source. The current source is used for the production of light by absorption of photons by transmission between the source and destination bands, and the diode is used to show the flow of the radiative recombination (the only mechanism permitted to recombination in detailed balance theory). By changing the place of the intermediate bands, the distance between the energy levels and therefore the production and radiative recombination currents will be changed.

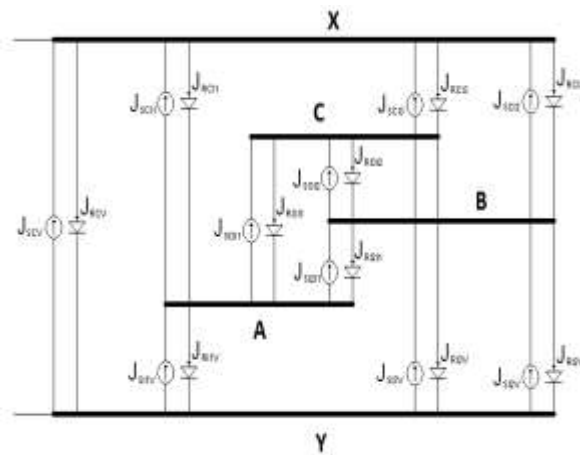


Fig. 1. The equivalent circuit model to simulate the solar cell with three intermediate bands.

To calculate the maximum efficiency for specific locations for intermediate bands, the production and recombination currents at nodes X and Y are calculated and the minimum current as a result of the current production of solar cells has been considered, and finally, the upper limit on the maximum power output and efficiency are achieved.

4. RESULTS AND DISCUSSION

The dimensions of Quantum dots in the direction of x and y (perpendicular to the main cell) are identical and 5.8 nm and for z-direction, it is assumed 3.5 nm. Also, the distance between the quantum dots in the directions x and y is identical to 20 nm and for z direction, between 20 to 300 nm is assumed. The distance between quantum dots along z, actually is the distance between the layers of quantum dots, and its change, due to the limited length of the cell, changes the number of layers of quantum dots. By creating layers of quantum dots, the distance between quantum dots in the direction of solar cell growth from a practical point is specific and dependent on the solar cell manufacturing process and cannot be involved in it, but by assuming that this distance can be changed, calculation of absorption coefficient is done until the impact of possible changes in the distance between the layers of the quantum dots in the upper limit of efficiency may be shown in its simplest form. In addition, the mole fraction for the material of quantum dots is assumed to be zero. To prove the validity of the method of calculation that is used, the absorption coefficient between the intermediate bands of the conduction region is calculated. The following curves show the variation of the absorption coefficient between intermediate bands of the conduction region for different polarization light. As be seen, the results with the results presented in [22] shown in Fig. 4 are similar well, and the validity of computational method is proved.

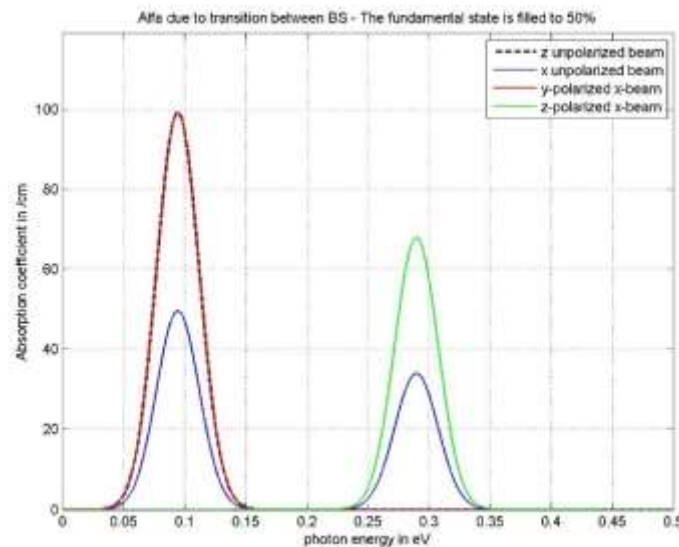


Fig. 2. Changes in the absorption coefficient between intermediate bands of conduction region for FF = 1.

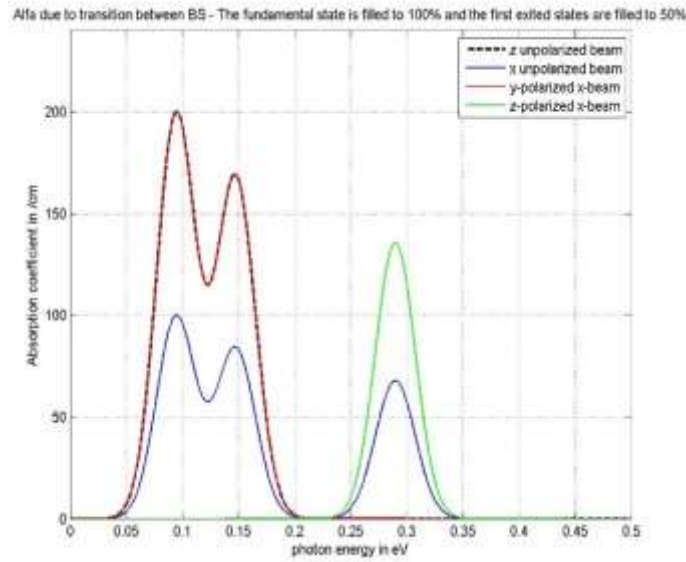


Fig. 3. Changes in the absorption coefficient between intermediate bands of conduction region for FF = 2.

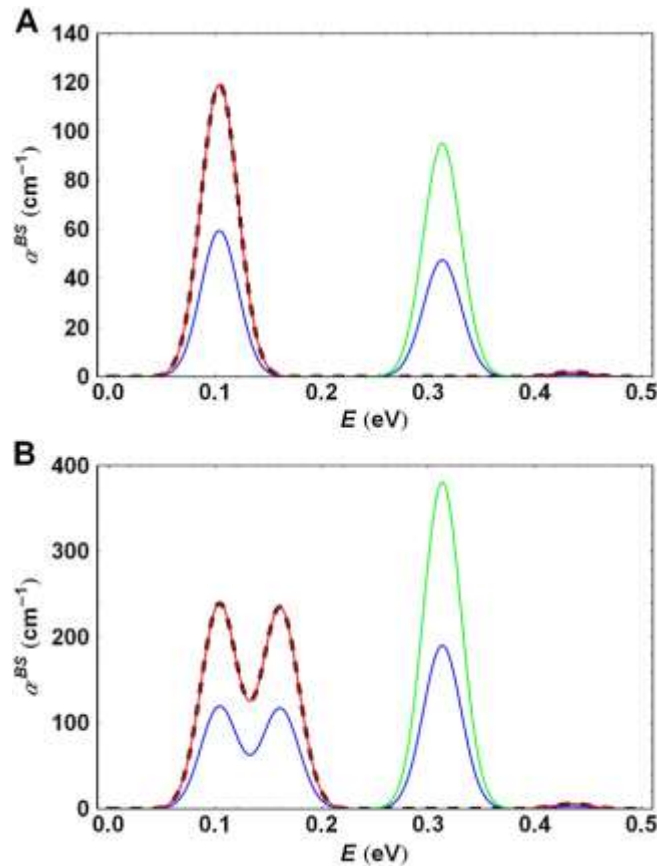


Fig. 4. The curve of the variation for absorption coefficient between the intermediate bands borrowed from [22]

To evaluate the effect of distance between quantum dot layers, we change the L_c parameter, which shows the period in z-direction or direction of light radiation, and for comparison, the sum of absorption coefficient in all desired energy spectrums is calculated and compared with each other.

Results are shown in the following figure:

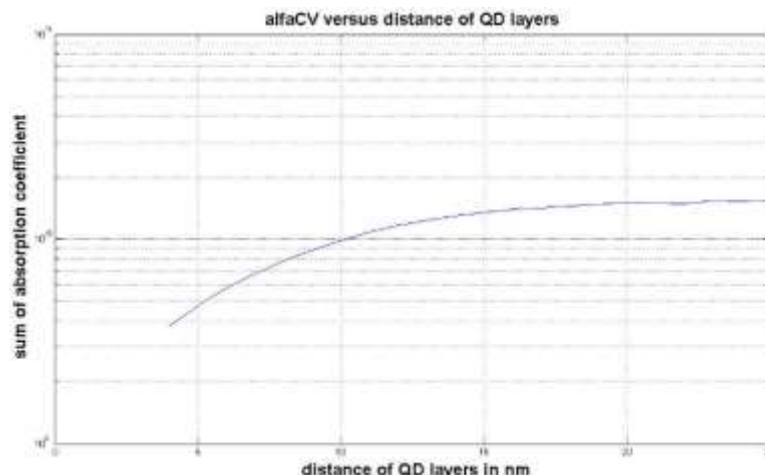


Fig. 5. Changes in the absorption coefficient per changes between quantum dot layers

As can be seen from the above figure, increasing the distance between quantum dot layers causes an increase in the absorption coefficient and follows the increasing efficiency of the solar cell.

Adding quantum dot layers to create intermediate bands in solar cells, results in the absorption of sub-bandgap photons on one hand, but on the other hand, follows the reduction of absorption coefficient in the transition between conduction bands and valance bands.

Therefore, we must balance the place of adding quantum dot layers and the number of them on one hand and the absorption coefficient in the transition between conduction and valance bands on the other hand.

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