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 in acceptable level. Actual results of using quantum dots have been led to decrease efficiency of solar cell. The effect of absorption coefficients on upper limit of efficiency in special type of solar cell is focus in this paper the main factors which have most impact on the upper limit of efficiency of our position of intermediate bands and consequently the structure of quantum dots. Furthermore, the changes in cell characteristics, quantum dots type, quantum dots structure, and even polarization of the incident light can change the upper limit of efficiency. Changes distances layers of quantum dots create different results for different polarization of light for 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 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 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, creation of energy levels due to the special doping with appropriate energy balance because of low level of concentration, don't have the characteristics of a band and despite allowing the absorption of low energy photons do not guarantee the 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 Highly mismatching dimension. 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 intermediate band using quantum dots can be a further increase in performance. In the first researches (for example [16]) actual results of using quantum dots were against the expected results because these changes cause to decreasing the solar cell efficiency. This reduction is contrary to the goals of the researchers then they decided to examine the reasons of this occurrence. Along with these researches, attention was paid to the absorption of photons in these structures, because in addition to solar cells [17-18], have 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 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 the section 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

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

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$$\alpha(E) = \frac{2\pi^2 e^2 E}{n_{ref} ch \varepsilon_0} \times \frac{|\langle \psi | r. \varepsilon | \psi \rangle|^2}{S} \times F N_l \delta(E - E_{line})$$
(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, N₁ is the number of QD layers per unit length, S is the Effective cross-sectional area of each quantum dot, and Eline is the energy difference between the two states. It should be noted that the density of quantum dots is equal to FNI / 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]:

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

 $\left| \left\langle \psi | \varepsilon . r | \psi' \right\rangle \right|^2$ 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 considered 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 In1-xGaxAs 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 dimension 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 is considered.

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

1- Z Unpolarized Beam: In this case, the light emitted in the direction z and light polarization vector that is perpendicular to the light beam can have any direction in the xy plane.

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- 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:

$$r = xi + yj + zk \tag{3}$$

$$\varepsilon = (\cos\phi\sin\theta)i + (\sin\phi\sin\theta)j + (\cos\theta)k \tag{4}$$

therefore:

$$\begin{aligned} \left| \langle \psi | \varepsilon, r | \psi' \rangle \right|^2 &= \cos^2 \varphi \sin^2 \theta \left| \langle \psi | x | \psi' \rangle \right|^2 \\ &+ \sin^2 \varphi \sin^2 \theta \left| \langle \psi | y | \psi' \rangle \right|^2 + \cos^2 \theta \left| \langle \psi | z | \psi' \rangle \right|^2 \end{aligned} \tag{5}$$

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

$$D_{t} = |\langle \psi | t | \psi' \rangle| = \int_{-l}^{l} \psi_{t}^{*} t \psi_{t}^{'} dt = A_{n} B_{m} \left(\frac{1}{(k_{m} + k_{n})^{2}} sin(l(k_{m} + k_{n})) - \frac{l}{k_{m} + k_{n}} cos(l(k_{m} + k_{n})) \right) + A_{n} B_{m} \left(\frac{1}{(k_{m} - k_{n})^{2}} sin(l(k_{m} - k_{n})) - \frac{l}{k_{m} - k_{n}} cos(l(k_{m} - k_{n})) \right)$$

$$(6)$$

Thus we have:

$$\left|\left\langle\psi\left|\varepsilon.r\right|\psi'\right\rangle\right|^{2} = \cos^{2}\phi\sin^{2}\theta \times D_{x}^{2} + \sin^{2}\phi\sin^{2}\theta \times D_{y}^{2} + \cos^{2}\theta \times D_{z}^{2}$$
(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:

$$\begin{aligned} \left| \langle \psi | \varepsilon. r | \psi' \rangle \right|^2 &= \cos^2 \varphi \sin^2 \theta \left| \langle \psi | x | \psi' \rangle \right|^2 + \\ \sin^2 \varphi \sin^2 \theta \left| \langle \psi | y | \psi' \rangle \right|^2 + \cos^2 \theta \left| \langle \psi | z | \psi' \rangle \right|^2 \\ &= A \left| \langle \psi | x | \psi' \rangle \right|^2 + B \left| \langle \psi | y | \psi' \rangle \right|^2 + C \left| \langle \psi | z | \psi' \rangle \right|^2 \end{aligned} \tag{8}$$

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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 that parity of its quantum number is different with respect to parity of source band. Thus, as seen in the following table if the parity of source band is odd the parity of destination band is even and vice versa.

The fullness of the intermediate band is effective in 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 was mentioned, the lowest intermediate band half-filled and other bands are assumed to be empty.

In the latter case with the FF = 2 in the charts was mentioned, 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 Figure 1 for a cell with three intermediate band is considered. Obviously, it will be extended to more or less the intermediate band.

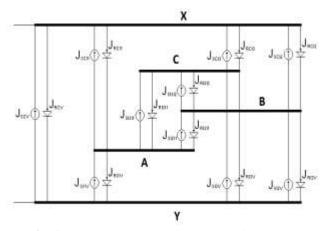


Fig. 1. The equivalent circuit model to simulate the solar cell with three intermediate bands.

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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 (only mechanism permitted to recombination in detailed balance theory). By changing the place of the intermediate bands, distance between the energy levels and therefore the production and radiative recombination currents will be changed.

To calculate the maximum efficiency for specific locations for intermediate bands, the production and recombination currents at nodes X and Y are calculated and minimum current as a result of 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 dimension of Ouantum dots in the direction of x and y (perpendicular to the main cell) is identical and 5.8 nm and for z direction 3.5 nm are assumed. Also distance between the quantum dots in the directions x and y identical to 20 nm and for z direction between 20 to 300 nm are 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, change the number of layers of quantum dots. By creating layers of quantum dots, the distance between quantum dots in 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 method of calculation that is used, the absorption coefficient between the intermediate bands of conduction region are 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] that shown in Figure 4 are similar well, and the validity of computational method is proved.

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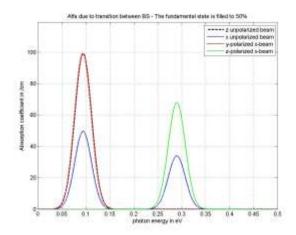


Fig. 2. Changes in the absorption coefficient between intermediate bands of conduction region for FF = 1.

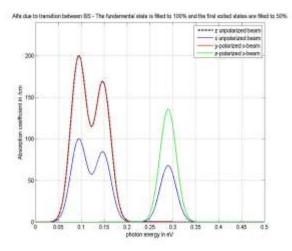


Fig. 3. Changes in the absorption coefficient between intermediate bands of conduction region for FF = 2.

To evaluate the effect of distance between quantum dot layers, we change the L_c parameter, that shows the period in z direction or direction of light radiation, and for comparison calculate the sum of absorption coefficient in all desired energy spectrum and compare them with each other.

Results are shown in the following figure:

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

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

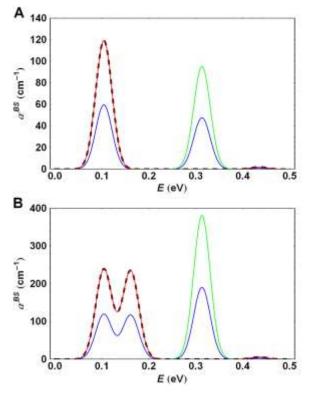
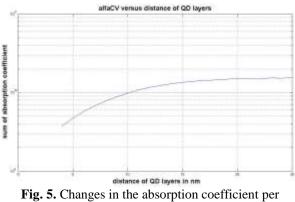


Fig. 4. The curve of the variation for absorption coefficient between the intermediate bands borrowed from [22].



changes between quantum dot layers.

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

REFERENCES

- Shockley W. & Queisser H. J. "Detailed balance limit of efficiency of p-n junction solar cells". J. Appl. Phys. 32, 510-519 (1961).
- [2] Luque A. & Marti A. "Increasing the efficiency of ideal solar cells by photon induced transitions at intermediate levels". Phys. Rev. Lett. 78, 5014-5017 (1997).

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- [3] J. Bruns, W. Seifert, P. Wawer, H. Winnicke, D. Braunig, and H. Wagemann, "Improved efficiency of crystalline silicon solar cells due to he+implantation". Applied Physics Letters, vol. 64, no. 20, pp. 2700–2, 1994.
- [4] M. J. Keevers and M. A. Green, Sol. Energy Mater. Sol. Cells 41 195 (1996).
- [5] H. Kasai, T. Sato, and H. Matsumura, "Impurity photovoltaic effect in crystalline silicon solar cells", in Conference Record of the Twenty Sixth IEEE Photovoltaic Specialists Conference - 1997 (Cat. No.97CB36026), 1997, pp. 215–18.
- [6] S. P. Bremner, R. Corkish, and C. B. Honsberg, "Detailed balance efficiency limits with quasi-fermi level variations", IEEE Transactions on Electron Devices, vol. 46, no. 10, pp. 1932–9, 1999.
- [7] L M. Green, "Prospects for photovoltaic efficiency enhancement using low-dimensional structures". Nanotechnology, vol. 11, no. 4, pp. 401–5, 2000.
- [8] K. Barnham, B. Braun, J. Nelson, M. Paxman, C. Button, J. Roberts, and C. Foxon, "Short-circuit current and energy efficiency enhancement in a low-dimensional structure photovoltaic device", Applied Physics Letters, vol. 59, no. 1, pp. 135–7, 1991.
- [9] A. Mart'ı, L. Cuadra, and A. Luque, "Quantum dot intermediate band solar cell", in Conference Record of the Twenty-Eighth IEEE Photovoltaic Specialists Conference, Anchorage, AK, USA, 2000, pp. 940–3.
- [10] A. Mart'ı, E. Antol'ın, C. Stanley, C.Farmer, N. L'opez, P. D'ıaz, E. C'anovas, P. Linares, and A. Luque, "Production of photocurrent due to intermediate-to-conduction-band transitions: A demonstration of a key operating principle of the intermediate-band solar cell", Physical Review Letters, vol. 97, no. 24, pp. 247 701/1-4, 2006.
- [11] A. G. Norman, M. C. Hanna, P. Dippo, D. H. Levi, R. C. Reedy, J. S.Ward, and M.M. Al-Jassim, "InGaAs/GaAs QD superlattices: MOVPE growth, structural and optical characterization, and application in intermediate-band solar cells", in Conference Record of the 31st IEEE Photovoltaic Specialists Conference, Orlando, FL, USA, 2005, pp. 43–8.
- [12] M. Y. Levy and C. Honsberg, "Nanostructured absorbers for multiple transition solar cells", IEEE Transactions on Electron Devices, vol. -, no. -, p. in print, 2008.
- [13] K. Yu, W. Walukiewicz, J.W. Ager III, D. Bour, R. Farshchi, O. Dubon, S. Li, I. Sharp, and E. Haller,

"**Multiband GaNAsP quaternary alloys**", Applied Physics Letters, vol. 88, no. 9, p. 092110, 2006.

- [14] W. Shan, W. Walukiewicz, J.W. Ager III, E. Haller, J. Geisz, D. Friedman, J. Olson, and S. Kurtz, "Band anticrossing in gainnas alloys", Physical Review Letters, vol. 82, no. 6, pp. 1221 – 4, 1999.
- [15] W. Walukiewicz, K. Yu, J. Wu, J.W. Ager III, W. Shan, M. Scrapulla, O. Dubon, and P. Becla, "Highly mismatched alloys for intermediate band solar cells", Thin-Film Compound Semiconductor Photovoltaics. Symposium (Materials Research Society Symposium Proceedings Vol.865), pp. 125– 30, 2005.
- [16] Luque, A., and Steven Hegedus. "Handbook of Photovoltaic Science and Engineering". Chichester, West Sussex, U.K.: Wiley, 2011. Print.
- [17] Martí A, Cuadra L, Luque A. "Quantum dot intermediate band solar cell". IEEE: Proc. 28th IEEE Photovoltaics Specialists Conference, New York, 2000.
- [18] Luque A, Martí A, Stanley C, López N, Cuadra L, Zhou D, Mc-Kee A. "General equivalent circuit for intermediate band devices: potentials, currents and electroluminescence". Journal of Applied Physics 2004; 96(1): 903–909.
- [19] Berryman KW, Lyon SA, Segev M. "Mid-infrared photoconductivity in InAs quantum dots". Applied Physics Letters 1997; 70(14): 1861–1863.
- [20] Liu HC, Duboz JY, Dudek R, Wasilewski ZR, Fafard S, Finnie P. "Quantum dot infrared photodetectors". Physica E: Low-dimensional Systems and Nanostructures 2003; 17: 631–633.
- [21] Luque A, Marti A, Antolin E, Garcia-Linares P. "Intraband absorption for normal illumination in quantum dot intermediate band solar cells". Solar Energy Materials and Solar Cells 2010; 94: 2032– 2035.
- [22] Luque A, Marti A, Mellor A, Fuertes Marron D, Tobias I & Antolin E. "Absorption coefficient for the intraband transitions in quantum dot materials". Prog. Photovolt: Res. Appl. (2012);
- [23] Luque A, Martí A, Antolín E, Linares PG, Tobías I, Ramiro I, Hernandez E. "New Hamiltonian for a better understanding of the quantum dot intermediate band solar cells". Solar Energy Materials and Solar Cells 2011; 95(8): 2095–2101.
- [24] Nozawa T. & Arakawa Y. "Detailed balance limit of the efficiency of multilevel intermediate band solar cells". Appl. Phys. Lett. 98, 171108 (2011).