# Optimal Location of the Intermediate Band Gap Energy in the Intermediate Band Solar Cell

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# **ABSTRACT:**

The purpose of this study is to determine the optimum location for intermediate band in the middle of band gap of an ideal solar cell for maximum performance. By changing the location of the intermediate band, output current and therefore performance can be changed. Choosing the best location in terms of solar cell energy gap and how to change the performance by means of the location of intermediate band has the important role in the energy band gap engineering. This matter in the known methods of the intermediate bands realization such as quantum well and quantum dots can be used for selecting the type of semiconductor in quantum well or quantum dot and also for selecting dimension of quantum dot or quantum well. Conclusion of this paper is by increasing energy gap, the optimal location of intermediate band for cells with one intermediate band, will be closer to the middle of the energy gap.

**KEYWORDS:** Band Position, Efficiency, Detailed Balance Theory, Maximum Efficiency.

#### **1. INTRODUCTION**

One of the major ways to improve the efficiency of solar cells is the intermediate bands. Add one or more intermediate in the band gap energy of the semiconductor solar cell substrate, in certain circumstances, can enhance its performance. By inserting one intermediate band in energy gap, three important transitions can be realize for absorption of a photon: (1)from valance band to intermediate band (2) from valance band to conduction band and (3) from intermediate band to conduction band. Several theoretical calculations carried out in this field represent an increase in the efficiency of solar cells with one intermediate band [1-5]. In fact, the intermediate band attracts less energetic photons and thus increases the efficiency of solar cells. For example, using the theory of detailed balance [1, 6], in the presence of an intermediate band, solar cell performance can be improve from 40% [1] to 60% [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. In practice, due to the lack of fulfillment of all the requirements, there is no corresponding increase in efficiency [7-8]. Some ways to create intermediate band gap energy of the semiconductor solar cell substrate include creating special doping with

appropriate energy balance [9-11], quantum wells [12-14], quantum dots [15-18] and highly mismatching alloys [19-21]. 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, but in quantum wells is in one dimension. Highly mismatching allovs. 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. Regardless of the creation method of the intermediate band, by expression the detailed balance theory components, our focus is on the optimal location of intermediate band gap energy in solar cells. Finding the optimal location of the intermediate band have the appropriate functional results in solar cell band gap engineering in each of realization methods of intermediate band.

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## 2. THEORETICAL BACKGROUND

According to the principle of detailed balance for a solar cell with one intermediate band is assumed: (1) Carrier transport mechanism between energy bands only radiation; (2) Carrier mobility is infinite; (3) No carrier is not outside, not inside the intermediate of the band; (4) Each photon carries the energy to participate in the transfer of energy between the bands to be absorbed; (5) Exit the radiation of recombination mechanism from the place of light entrance is possible; (6) We shall assume that for every range of energies only one of the three absorption lengths is important; (7) Cell light is isotropic. Simple schema model that is used for intermediate band solar cell is shown in Fig. 1.



**Fig. 1.** A simplified view of the pattern of the energy bands in intermediate band solar cell.

To facilitate the absorption of lower energy photons, in this pattern that one intermediate band in the energy gap is present, it is assumed that the main gap is divided into two smaller gap, and valence band is completely full, conduction band is completely empty and intermediate band is half full. Also it is assumed that in addition to the absorption of a photon between energy bands, on the principle of detailed balance, the photon emission of radiation recombination exist.

Absorption and emission, respectively, by diode and current source, shown in Fig. 2, has been modeling.



Fig. 2. Equivalent circuit model of solar cell by considering the absorption and emission between energy bands.

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In this model it is assumed that: (a) the sun radiation is like the black-body radiation at a temperature of 6000K; (b) Photon radiation from the recombination radiation in cells is like the black-body radiation at ambient temperature; (c) The density of photons emitted from the black body are obtained from the following equation:

$$F_{BB}(E_{l}, E_{h}, T) = [2\pi/(h^{3}c^{2})]$$
(1)  
 
$$\cdot \int_{E_{l}}^{E_{h}} E^{2}/(\exp(E/(k_{B}T)) - 1)dE$$

(d) According to the principle of detailed balance, the density of photons emitted by the light of the solar cell can be obtained from the following equation, which  $\mu$  is the chemical potential of the irradiated cells:

$$F_{BB}(E_{l}, E_{h}, \mu, T) = [2\pi/(h^{3}c^{2})]$$
(2)  
 
$$\cdot \int_{E_{l}}^{E_{h}} E^{2}/(\exp((E-\mu)/k_{B}T) - 1)dE$$

Current-voltage relationship for solar cells using the principle of detailed balance is:

$$J(V) = qf_{s}[F_{BB}(E_{G}, \infty, 0, T_{s}) + F_{BB}(E_{H}, E_{G}, 0, T_{s})] + q(f_{C} - f_{s})[F_{BB}(E_{G}, \infty, 0, T_{C}) + F_{BB}(E_{H}, E_{G}, 0, T_{C})] - qf_{c}[F_{BB}(E_{G}, \infty, \mu_{CV}, T_{C}) + F_{BB}(E_{H}, E_{G}, \mu_{IV}, T_{C})]$$
(3)

In which f<sub>C</sub>=1, f<sub>S</sub>=X.sin<sup>2</sup> $\theta_{sun}$ =X × 2.1646×10<sup>-5</sup>, 1≤X≤ (sin<sup>2</sup> $\theta_{sun}$ )<sup>-1</sup>=46050 is light concentration factor and  $\theta_{sun}$ =0.26° is the angle of the sun from the cell; (e) given the need outflow failure carrying of intermediate band and not entering into its carrier, the following equation holds:

$$qf_{s}[F_{BB}(E_{L}, E_{H}, 0, T_{S}) + F_{BB}(E_{H}, E_{G}, 0, T_{S})] + q(f_{C} - f_{S})[F_{BB}(E_{L}, E_{H}, 0, T_{C}) + F_{BB}(E_{H}, E_{G}, 0, T_{C})] - qf_{C}[F_{BB}(E_{L}, E_{H}, \mu_{CI}, T_{C}) + F_{BB}(E_{H}, E_{G}, \mu_{IV}, T_{C})] = 0$$
(4)

This relation in other word is the current law in intermediate band node.

In degeneration conditions (  $E-\mu >> k_B T$  ) the following approximation can be used:

$$\left[\exp\left(\frac{E-\mu}{k_bT}\right)-1\right]^{-1} \approx \exp\left(\frac{\mu}{k_bT}\right)\left[\exp\left(\frac{E}{k_bT}\right)-1\right]^{-1}$$
(5)

As a result, components of relations (3) and (4) can be simplified as follows:

$$F_{BB}(E_{G}, \infty, \mu_{CV}, T_{C}) \approx F_{BB}(E_{G}, \infty, 0, T_{C}) \exp\left(\frac{\mu_{CV}}{k_{B}T}\right)$$

$$F_{BB}(E_{H}, E_{G}, \mu_{IV}, T_{C}) \approx F_{BB}(E_{H}, E_{G}, 0, T_{C}) \exp\left(\frac{\mu_{IV}}{k_{B}T}\right)$$

$$F_{BB}(E_{L}, E_{H}, \mu_{CI}, T_{C}) \approx F_{BB}(E_{L}, E_{H}, 0, T_{C}) \exp\left(\frac{\mu_{CI}}{k_{B}T}\right)$$
(6)

By replacing (5) in (3) and (6) the reason of using the diode model for radiation can be explained.

# 3. CALCULATION METHOD

By attention to Fig. 1 the following relations between chemical potentials and energy difference between difference bands can be obtained:

$$\begin{pmatrix} \mu_{N} \\ \mu_{CV} = \frac{E_{H}}{E_{G}} &, \quad \frac{\mu_{CI}}{\mu_{CV}} = \frac{E_{L}}{E_{G}} \end{pmatrix} , \quad (\mu_{CV} = \mu_{CI} + \mu_{N} &, \quad E_{G} = E_{H} + E_{L})$$
(7)

Therefore using light concentration factors : 1, 10, 100, 1000, 10000 and 46200 and changing energy gap from 0.5 to 5 electron volt and varying coefficient  $n=\mu IV/\mu CV$  from 0.5 to 0.9, maximum output power variation curves can be obtained. Because of symmetry, the results for changing n from 0.1 to 0.5 are identical to 0.5 to 0.9. In other words two optimum places exist for intermediate band, one in upper part of energy gap and the other in lower part of energy gap, and these two places are symmetry with respect to middle of energy gap. The results in the Fig.s of 3 to 7 can be seen.



**Fig. 3.** Variation of optimum place for intermediate band with respect to energy gap variation in different light concentration coefficients.

As be seen in Fig. 3, with increasing energy gap, the optimal place for intermediate band, moves to the center of the energy gap and depending on how the curve changes, it can be expected that the best place for

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intermediate band for infinite energy gap is the middle of energy gap.

For a closer look at the changes in the vicinity of the optimum performance shown in Fig. 3, we review the results in Fig. 4.



**Fig. 4.** Variation of efficiency with respect to variation of intermediate band place in different energy gap.

As be shown in Fig. 4, for each value of the energy gap, by changing the location of the intermediate band from the middle of gap to the conduction band, at first the efficiency increase and after reaching its maximum, which is the optimum place, the downside of it. Another thing that can be seen in the above Fig. is by increasing the energy gap; the gradient of the efficiency becomes higher that means in higher energy gap by changing the place of intermediate band the efficiency varies faster than lower energy gap. By increasing the light concentration coefficient doesn't have additional result and the results are the same as low light concentration coefficient. For example for X=10000 and X=46200 the results are shown in Fig.s 5 and 6.



Fig. 5. Variation of efficiency with respect to variation of intermediate band place in different energy gap for X=10000.



Fig. 6. Variation of efficiency with respect to variation of intermediate band place in different energy gap for X=46200.

# 4. RESULTS AND DISCUSSION

The results have the following implications:

- 1) There are two locations to ensure maximum performance is optimized for intermediate band.
- 2) The optimal location is near the center of the band gap energy.
- 3) The changes in maximum power output and consequently for maximum performance out of the optimized position for intermediate band is extremely high.

Results of the simulation studies show that the place of intermediate band has the main effect on achieving to maximum efficiency. Therefore changing the intermediate band from the optimum location can dramatically reduce the performance. Another main result is in the case of solar cells with one intermediate band, by increasing the energy gap the optimum location of intermediate band closes to the middle of energy gap.

## 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).
- [3] Andrew S. Brown and Martin A. Green "Intermediate band solar cell with many bands: Ideal performance". J. Appl. Phys. 94, No. 9, (2003).
- [4] Luque A. Linares P. G. Antolin E. Canovas E. Farmer C. D. Stanley C. R. and Marti A. "Multiple levels in intermediate band solar cells". Appl. Phys. Lett. 96, 013501 (2010).

- [5] Nozawa T. and Arakawa Y. "Detailed balance limit of the efficiency of multilevel intermediate band solar cells" Appl. Phys. Lett. 98, 171108 (2011).
- [6] Henry C. H., J. Appl. Phys. 51, 4494, (1980).
- [7] Luque A. and Marti A. "Photovoltaics: Towards the intermediate band". Nature Photon. 5, 137-138 (2011).
- [8] Luque A. Marti A. and Stanley C. "Understanding intermediate band solar cells" Nature Photon. 5, 146-152 (2012).
- [9] 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.
- [10] M. J. Keevers and M. A. Green, Sol. Energy Mater. Sol. Cells 41 195 (1996).
- [11] 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.
- [12] 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.
- [13] M. Green, "Prospects for photovoltaic efficiency enhancement using low-dimensional structures," Nanotechnology, vol. 11, no. 4, pp. 401–5, 2000.
- [14] 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.
- [15] 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.
- [16] 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.
- [17] 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.
- [18] M. Y. Levy and C. Honsberg, "Nanostructured absorbers for multiple transition solar cells," IEEE Transactions on Electron Devices, vol. -, no. -, p. in print, 2008.
- [19] 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.

- [20] 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.
- [21] 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.