PROGRESS IN IDEAL MODELS OF QUANTUM WELL SOLAR CELLS

A.K.Agarwal[1] , D.R. Mehrotra[2]

[1] *Dept. of Physics, Government College, Nasirabad, Ajmer (India)*

[2] *Dept. of Physics, Government College, Kishangarh, Ajmer (India)*

ABSTRACT

Quantum well solar cells (QWSC's) is a new approach toward high efficiency solar cells. In this paper we have discussed some ideal models of QWSC's based on Shockley's ideal equation for p-n junction. These models have shown efficiency enhancements in QWSC's qualitatively in certain limits. Models have good consistency with experimental results, and may be used for fabrication of QWSC from different materials. Finally, we have discussed shortcoming of these models and proposed how these model can be improved.

Keywords - *Quantum Well Solar Cells, Ideal Model, Efficiency Enhancement*

I. INTRODUCTION

Solar cells are the best option as alternative energy source. However, their limited efficiency (up to 20%) is a major obstacle in their utilization in a large scale power generation. In 1990,Barnham and his coworkers suggested that [1] multi-quantum-well (MQW) is a new approach to high efficiency solar cells which could surpass the 50% mark. Barnham et.al in Imperial College London, demonstrated experimentally that by inserting quantum wells in the intrinsic region of p-i-n solar cells the conversion efficiency could be enhanced [2].In the initial experiments at Imperial College, the photovoltaic properties of multiple-quantum-well (MQW) solar cells were compared to p-i-n solar cells with no quantum wells. The MQW devices exhibited significantly larger short-circuit currents and slightly lower open circuit voltages under illumination with a broadband light source. The maximum power conversion efficiencies were found more than double in presence of MQW.

Corkish and Green, [3] considered recombination and its effect on open circuit voltage in a theoretical study of quantum well cells, suggested that such enhancement is only significant for cells in which the host material band gap is greater than the optimum gap for a homojunction cell. After that, with detailed balancing theory, Araujo and Marti [4, 5] argued that inclusion of quantum wells in solar cells should not yield efficiencies higher than those theoretically possible for optimum single-gap cells.Imperial college group immediately challenged Araujo and Marti's argument with their experimental results [6, 7, 8] showing enhancement in the efficiency of QWSC's and they argued that their observation of quasi-fermi level variation suggest that spatially constant fermi level assumption made by Arujo and Marti is not applicable to QWSC.

Thus, QWSC have demonstrated some important aspects. However, a broad qualitative understanding has yet to emerge concerning trends in the terminal characteristics of QWSC.The work on QWSC is still in its infancy and much is yet to be unearthed.

Many theoretical models have been developed to explain the performance of MQW solar cells. These models have emphasized on effect of recombination on dark currents and open circuit voltage. In this article, different theoretical models for QWSC based on ideal current voltage relationship are discussed. The first model under consideration is [9], in which a complete absorption for all photons with energy greater than well band gap is assumed and most of the calculation is performed in the radiative limit. Rimada and Hernandez's model is an extension of Anderson's model in which assumption of complete absorption has been removed and it also accounted for well barrier recombination. Later, Lade and Zahedi revised and extended the ideal model by revising the equation for absorption flux and by revising the material data used. Finally we take into consideration the revised model given by Rimada et.al according to which insertation of multi quantum wells into depletion region of a p-i(MQW)-n AlGaAs solar cell can enhance the conversion efficiency. To sum up, we discuss the limitation of these models and propose the possible improvements in it.

II. ANDERSON MODEL

The first ideal analytical model for quantum well solar cells, based on Shockley equation for p-n junction, was presented by Anderson [9]. The model explicitly included the contribution of both generation and recombination of carriers in QWSC in ideal p-n junction equation. According to this model, the J(V) relation for base line p-i-n solar cell of band gap E_B is given by:

$$J_B(V) = J_0(1+\beta)\left[\exp(qV/kT)-1\right] - q\Phi_B \qquad (1)$$

Where $$\beta = \frac{qWB_B n_{iB}^2}{J_0} \qquad (2)$$

Here q is the electron charge, V is the terminal voltage, kT is the thermal energy, J_0 is the reverse saturation current density, W is the intrinsic region width, B_B is the barrier recombination coefficient, and Φ_B is the net flux of incident photons with energies greater than or equal to E_B. n_{iB} is the equilibrium intrinsic carrier concentration for the baseline cell material and β is the ratio of the current required to feed radiative recombination in the intrinsic region at equilibrium to the usual reverse drift current resulting from minority carrier extraction.

Similarly, he considered a quantum well solar cell in which a fraction f_w of the intrinsic region volume was replaced by quantum well material of band gap $E_A\,(E_A < E_B)$. With these modification the $J(V)$ relation for the quantum well cell is given as:

$$J_{QW}(V) = J_0(1+r_R\beta)\left[\exp(qV/kT)-1\right] - qr_G\Phi_B \qquad (3)$$

Here, $\Delta E = E_B - E_A$

In above relation, generation enhancement ratio r_G and the radiative enhancement ratio r_R were defined as follows:

$$r_G = \frac{\Phi_A}{\Phi_B} \qquad (4a)$$

$$r_R = 1 + f_W\left[\gamma_B\gamma_{DOS}^2\exp(\Delta E/kT) - 1\right] \quad (4b)$$

Here, similarly to Φ_B, Φ_A is the net flux of incident photons with energies greater than or equal to E_B and another parameters γ_B and γ_{DOS} were defined as oscillator enhancement factor anddensity-of-states enhancements factor respectively.

Anderson compared base line model to quantum well model in the limit where all incident photons with energies above the lowest band gap in the cell are absorbed in the intrinsic region and gave the relation as

$$J_{QW}(V) = J_B(V) + \left\{J_0(r_R - 1)\beta\left[\exp(qV/kT) - 1\right] - q(\Phi_A - \Phi_B)\right\} \quad (5)$$

Anderson analyzed these expressions with available material parameters theoretically and has shown that in terminal characteristics of quantum well solar cells only band gap is significant.The short circuit current depends only on the lowest band gap in the structure i.e. quantum well band gap.As the quantum wells are deepened, the short-circuit current increases due to the additional carrier generation in the wells (increasing r_G) while the open-circuit voltage is reduced from the additional recombination (increasing r_R). The open-circuit voltage, however, will be relatively unaffected for small values of Δ*E* where $r_R\beta << 1$ so $(1+\beta) \sim (1 + r_R\beta)$. Thus, in the small Δ*E* regime, the maximum possible value of *J*(*V*)*V* is increased by the presence of the quantum wells and the conversion efficiency is enhanced. Above some value of Δ*E*, however, the exponential dependence of r_R on Δ*E* will rapidly force $r_R\beta >> 1$ with increasing Δ*E*, thus lowering the open-circuit voltage with increasing Δ*E* and limiting the maximum conversion efficiency. The band gap difference Δ*E* at which quantum well recombination becomes important can be estimated by solving $r_R\beta = 1$ for Δ*E*, which was given as:

$$\Delta E' \equiv \frac{kT}{q}\ln\left(\frac{1-\beta(1-f_w)}{\beta f_w\gamma_B\gamma_{DOS}^2}\right) \quad (6)$$

Thus, Anderson model predicts that efficiency enhancement is possible through the introduction of quantum wells and that the conversion efficiencies for quantum well can be higher than that of the optimum base line cell.

III. RIMADA-HERNANDEZ'S MODEL

Anderson considered that the light is absorbed in the quantum wells of continuous form and not through discrete levels of energy as it really happens. J.C. Rimada and L. Hedrnandez [10, 11] suggested that above approximation leads to the overestimation of the photocurrent. Thus, they gave another ideal model by removing the complete absorption assumption and accounting for well / barrier inter face recombination. Rimada-Hernandez have shown that the insertion of MQW into the depletion region of a p-i(MQW)-n $Al_xGa_{1-x}As$ solar cell can significantly enhance the conversion efficiencies.

Similar to Andersons's model,Rimada and Hernandez's model was also based on well-known p-n junction equation for ideal diode,Rimada et-al added a non-radiative current density term in carrier generation current density expression presented in Anderson's model. The *J*(*V*) relation for the ideal homogeneous p-i-n solar cells was given as:

$$J(V) = J_0(1+\beta)\left[\exp(qV/kT)-1\right] + J_1\left[\exp(qV/2kT)-1\right] - q\Phi_B \quad (7)$$

Where $J_1 = qWA_B n_\infty B$ is the nonradiative Auger current.

Rimada and Hernandez substituted intrinsic region of $Al_xGa_{i-x}As$ solar cell with MQW material with lower Al composition and modified J(*V*) relationfor MQW solar cells as

$$J_{MQW} = J_0(1+r_R\beta)\left[\exp(qV/kT)-1\right] + (J_1 r_{NR} + J_s)\left[\exp(qV/2kT)-1\right] - qW\Phi \quad (8)$$

Here non radiative enhancement ratio *Rnr*, and superficial recombination current *Js* were introduced first time. These parameters were defined as

$$r_{NR} = 1 + f_w\left[\gamma_A\gamma_{DOS}\exp\{(\Delta E/2kT)-1\}\right] \quad (9a)$$

$$J_s = 2Nqn_{iB}v_s\gamma_{DOS}\exp(\Delta E/kT) \quad (9b)$$

Where γ_A and v_s are lifetime reduction factor andthe superficial recombination rate at interfaces respectively.

Rimada and Hernandez calculated the flux absorbed in the barriers in the presence of an AM1.5 spectral photon flux $N_{ph}(E)$ as

$$\phi_B = \int_{E_B}^{\infty} N_{ph}(E)\exp\left[\alpha_B(E)W\right]dE \quad (10)$$

And the flux absorbed per well as

$$\phi_w = \sum_n N_{ph}(\lambda_n)\exp\left[\alpha_w(\lambda_n)L_W\right]\Delta\lambda_n \quad (11)$$

Where the summation is performed over all permitted transitions λ_n, with linewidths $\Delta\lambda_n$. Here $\alpha_B(E) > 0$ and $\alpha_W(\lambda_n) > 0$ are the barrier and well absorption coefficients, respectively. The total flux absorbed is then calculated as

$$\phi = \Phi_B + N_W\Phi_W \quad (12)$$

They computed conversion efficiency of MQW solar cells by varying barrier band gap energy and superficial recombination rates and found that for the interface recombination rate of $v_s \le 165\,cm/s$, the p-i(MQW)-n solar cells enhance the short-circuit current sufficiently to overcome the voltage loss and so it ensures that the conversion efficiency is always higher than the conventional p-i-n solar cells.The Rimada and Hernandez model exhibits efficiency enhancement of MQW solar cells.

3.1 LADE AND ZAHEDI MODEL

Lade and Zahedi [12] found that the absorption in Rimada et-al model was overestimated therefore, they revised and extended the ideal model by revising the equation for absorbed flux by introducing expression to compute accurately the well effective densities of states and the radiative recombination coefficients and by revising the material data used. The model though, assume constant quasi fermi level separation and its results are consistent with the theory of detailed balance[4, 5].

Lade and Zahedi considered that the absorption spectrum is stepped as suggested by Bastard's [13]. They gave the well absorption coefficient for the nth heavy hole transition using Bastard's expression as

$$\alpha_{e_n-hh_n}(E) = \frac{\pi q^2 E_p}{4\pi\varepsilon_0 n_r c\, m_0 E \ell \hbar} \frac{m_{e,W_{xy}} m_{hh,W_{xy}}}{m_{e,W_{xy}} + m_{hh,W_{xy}}} Y(E - E_n) \tag{13}$$

Where Y is the step function and ℓ is the 'quantum thickness of the hetero structure' [13]. By considering the well absorption spectrum continuous rather than discrete, Lade and Zahedi gave a more appropriate expression to calculate the total absorbed flux as

$$\phi = \int_{E_a}^{\infty} N_{ph}(E)\left[1 - \exp\left(-\alpha_B(E)\right)W - N_W \alpha_W(E)\ell\right] dE \tag{14}$$

The material data for AlGaAs /GaAs, as referred. [14 - 25],were used by Lade and Zahedi to evaluate open circuit voltage and short circuit current. They revised density of states calculations by following the derivation of Nelson et al. [26] under the additional assumption that the energy of all carriers exceeds their respective quasi-fermi levels by many multiples of *kT*. They also use expression for current density due to radiative recombination from detailed balance theory [4]. Which was given by,

$$J_{rad}(V) = q\int_0^{\infty} F(E)\, b_n(E, qV, T)\, dE \tag{15}$$

Where $F(E)$ accounts for the emissivity and geometrical factors and $b_n(E, qV, T)$ is the blackbody spectrum in a medium of refractive index n for an emitter at temperature T with quasi-Fermi level separation qV. With revised data and expressions, they compared the experimental results for the cells of Aperathitis et al. [27] with the predictions of Rimada's and their model. Experimental comparison showed that the Lade and Zahedi model correctly predicts the results for single gap cell to MQW cells.

Thus, Lade and Zahedi's model also showed that efficiency enhancements are achievable for AlGaAs/GaAs even in detailed balance theory assumptions.

IV. IMPROVED RIMADA'S MODEL

Rimada and his co-researcher's extended their previous model for QWSC'sin which both barrier and well materials are made of AlGaAs[28, 29]. In this model the cell materials were $Al_X Ga_{1-X} As$ for the host cell and barriers and $Al_Y Ga_{1-Y} As$ for the wells, where $0 \le y \le x \le 0.35$, in order to ensure minor gap for the well material and direct gap.Rimada et al studied conversion efficiency as a function of Al composition in barrier and wells. Rimada et al revised current voltage relationship of the MQW cell as given in their previous model with modifying current density due toabsorption of photon by QWSC.The modified J-V relation for MQW was given by:

$$J_{MQW} = J_0 (1 + r_R \beta) \left[\exp\left(\frac{qV}{kT} \right) - 1 \right] + (\alpha r_{NR} + J_S) \left[\exp\left(\frac{qV}{2kT} \right) - 1 \right] - J_{PH} \qquad (16)$$

The photocurrent J_{PH} was calculated from the integration of external quantum efficiency of the cell (QE) over solar spectrum $F(\lambda)$ in AM1.5 solar radiation [30],

$$J_{PH} = q \int F(\lambda) QE_{TOTAL}(\lambda) d\lambda \qquad (17)$$

Here QE values is calculated by the expression

$$QE(\lambda) = [1 - R(\lambda)] \exp\{(-\sum \alpha_i z_i)[1 - \exp(-\alpha_B W - N \alpha_W^*)]\} \qquad (18)$$

where $R(\lambda)$ is the surface reflectivity spectrum, the first exponential factor is due to the attenuation of light in the precedent layers of the cell, α_i and z_i are the absorption coefficient and the width of the precedent layers, respectively, the α_B is the absorption coefficient of the bulk barrier material, N is the number of wells and α_W^* is the non-dimensional quantum well absorption coefficient, used for energies below the barrier band gap.

Rimada and co-worker's compare and calculate QE with available experimental results and found agood agreement between modeled and experimental QE spectra. The dependence of conversion efficiency on quantum well and baseline band gap was examined as a function of Al composition of barrier (x_B) and well (x_W) in the AlGaAs QWSC. They found that with well width of 15 nm and 15 wells efficiency reached to maximum which was approximately 20% higher than and its equivalent baseline cell. It was also found that there is a wide range of Al composition barrier $(0.05 < x_B < 0.3)$ and Al composition well $(0 < x_W < x_B)$ where the QWSC efficiency is alwayshigher than corresponding homogeneous p-i-n cell without quantum wells.Rimada et al concluded that upto 15 wells in intrinsic region of QWSC's would show efficiency enhancements over base line cell.

V. CONCLUSION AND SCOPE FOR FUTURE WORK

Barnham and Co-workers proposed MQW as a novel approach to high efficiency-solar cells. However,some researchers have created a controversy whether the QWSC conversion efficiency would reach beyond that of the base line bulk device of optimal band gap in case of radiative recombination dominance. Numbers of experiments have shown that efficiency enhancement is possible in QWSC's but how to achieve such enhancements in real practical solar cells depends upon its optimized design. Thus, presently researchers are targeting to predict the behavior of QWSC's for optimizing the design.

In this article we have discussed theoretical models based on current voltage relationship of ideal *p*-*n* junction to explain the performance of the QWSC's. Anderson presents first ideal model in which he showed that by introducing MQW material into the intrinsic region of a *p*-*i*-*n* solar cell the efficiency could be enhanced. He considered continuous absorption of light in quantum wells thus, his model overestimate the photocurrent in quantum well solar cell. Rimada and Hernandez extended this model by removing the complete absorption assumption and accounting for well / barrier interface recombination. Their model showed a critical dependence of efficiency on a quantum well depth. In Rimada's model exponential factor in absorption flux is evaluated to more than unity which lead to higher value of absorption flux. This inconsistency was removed in Lade and Zahedi's model. They presented another improved model by revising expression for absorption flux and material data. Prediction of this model appeared more consistent with experimental results.Rimada etal improved their previous model in which they vary Al composition in barrier and well and determined that for QWSC of AlGaAs there is wide range of Al composition barrier for which QWSC efficiency is always higher than homogenous *p*-*i*-*n* solar cells. They showed that the efficiency of QWSC's is more than baseline cells until the 15 wells in intrinsic region.

These models provide a basic approach for optimizing the design of QWSC's of AlGaAs. In future,if these models are applied to other solar cells material like InGaAsP etc, we may find better scenario of QWSC's design. Lade and Zahedi's model has shown efficiency enhancement in constant quasi Fermi level assumption. This assumption has already been questioned by number of experiments. Thus, if the model is revised with small quasi fermi level variation, the results will be more realistic. Another most important shortcoming of these models is radiative recombination, which is assumed as dominating recombination process. The Shockley – Read – Hall recombination is an important process in p n junction. Thus, Ideal model may be revised with SRH recombination for better consistency.

REFERENCES

[1] K. W. J. Barnham, C. Duggan, A new approach to high-efficiency multi-band gap solar cells. J. Appl. Phys. 67 (7) (1990) 3490-3493.

[2] K. W. J. Barnham, B. Braun, J. Nelson, M. Paxman, C. Button, J. S. Roberts, C. T. Foxon, Short-circuit current and energy enhancement in a low-dimensional structure photovoltaic device, Appl. Phys. Lett. 59 (1) (1991) 135-137.

[3] R. Corkish and M. A. Green, Proceedings of the 23rd IEEE Photovoltaics Specialists Conference, 1993, 99. 675-680.

[4] G. L. Araujo, A. Marti, Absolute limiting efficiencies for photovoltaic energy conversion, Sol. Energy Mater. Sol. Cells 33 (2) (1994) 213-240.

[5] G. L. Araujo, A. Marti, F. W. Ragay, and J. H. Wolter, Proceedings of the 12th EC Photovoltaic Solar Energy Conference, Amsterdam, April 11-15 1994, 9. 1429.

[6] K. W. J. Barnham, J. P. Connolly, N. Ekins-Daukes, B. Kluftinger, J. Nelson, C. Rohr, Recent results on quantum well solar cells, J. Mater, Sci. Mater. Electron. 21 (2000) 531-536.

[7] K. W. J. I. Ballard, J. P. Connolly, N. J. Ekins-Daukes, B. G. Kluftinger, J. Nelson, C. Rohr, Quantum well solar cells, Physica E 14 (2002) 27-36.

[8] J. Nelson, K. Barnham, J. Connolly, G. Haarpaintner, C. Button, and J. Roberst, Proceedings of the 12th CE Photovoltaic Solar Energy Conference, Amsterdam, April 11-15 1994, p. 1370.

[9] N. G. Anderson, Ideal theory of quantum well solar cells, J. Appl. Phys. 78 (3) (1995) 1850-1861.

[10] J. C. Rimada, Modelacion de celdassolares p-i-n de $Al_xGa_{1-x}As$ con pozoscuanticos en la region intrinseca, MSc Thesis, Universidad de la Habana, 2000.

[11] J. C. Rimada, L. Hernandez, Modelling of ideal AlGaAs quantum well solar cells, Microelectron. J. 32 (9) (2001) 719-723.

[12] S. J. Lade, A. Zahedi, A revised ideal model of AlGaAs/GaAs quantum well solar cells, Microelectron. J. 35 (5) (2004) 401-410.

[13] G. Bastard, Wave mechanics applied to semiconductor heterostructures, Les Editions de Physique, Les Ulis, 1988.

[14] F. H. Pollak, Energy gaps of AlGaAs (1992), in: S. Adachi (Ed.), Properties of Aluminium Gallium Arsenide, INSPEC, London, 1993. 53-57.

[15] M. L. Timmons, Surface and interface recombination velocities in AlGaAs (1992), in: S. Adachi (Ed.), Properties of Aluminium Gallium Arsenide, INSPEC, Londonm 1993, 235-237.

[16] M. Missous, Conduction and valence band offsets at the GaAs/AlGaAsheterostructure interface (1991), in: S. Adachi (Ed.), Properties of Aluminium Gallium Arsenide, INSPEC, London, 1993, 73-76.

[17] S. Adachi, Electron effective mass in AlGaAs (1991), in: S. Adachi (Ed.), Properties of Aliminium Gallium Arsenide, INSPEC, London, 1993, 58-65.

[18] S. Adachi, Hole effective mass in AlGaAs (1991), in: S. Adachi (Ed.), Properties of Aluminium Gallium Arsenide, INSPEC, London, 1993, 66-72.

[19] D. D. Nolte, Table of GaAs optical function at 300 K, in: M.R. Brozel, G.E. Stillman (Eds.), Properties of Gallium Arsenide, third ed., INSPEC, London, 1996, 207-213.

[20] M. Paxman, J. Nelson, B. Braun, J. Connolly, K. W. J. Barnham, C. T. Foxon, J. S. Roberts, Modeling the spectral response of the quantum well solar cell, J. Appl. Phys. 74 (1) (1993) 614-621.

[21] H. C. Hamaker, Computer modeling study of the effects of inhomogeneous doping and/or composition in GaAs solar-cell devices, J. Appl. Phys. 58 (6) (1985) 2344-2351.

[22] S. R. Wenham, M. A. Green, M. E. Watt, Applied Photovoltaics, Centre for Photovoltaics Devices and Systems, Sydney, 1994.

[23] J. Nelson, Quantum well solar cells, in: M. D. Archer, R. Hill (Eds.), Clean Electricity from Photovoltaics, Imperial College Press, London, 2001, (Chapter 10).

[24] J. Nelosn, I. Ballard, K. Barnham, J. P. Connolly, J. S. Roberts, M. Pate, Effect of quantum well location on single quantum well p-i-n photodiode dark currents, J. Appl. Phys. 86 (10) (1999) 5898-5905.

[25] R. K. Ahrenkiel, Minority-carrier lifetime and diffusion length in AlGaAs (1992), in: S. Adachi (Ed.), Properties of Aluminum Gallium Arsenide, INSPEC, London, 1993, pp. 221-224.

[26] J. Nelson, M. Paxman, K. W. J. Barnham, J. S. Roberts, C. Button, Steady-state carrier escape from single quantum wells, IEEE J. Quantum. Electron. 29 (6) (1993) 1460-1467.

[27] E. Aperathitis, Z. Hatzopoulos, M. Kayambaki, V. Foukaraki, M. Ruzinsku, V. Saly, P. Sirotnu, A. C. Varonides, P. Panyaotatos, 1 cm × 1 cm GaAs/AlGaAs MQW solar celsl under one sun and concentrated sunlight, 28th IEEE Photovoltaics Specialists Conference, Anchorgae, IEEE Press. Piscataway, 2000, pp. 1142-1145.

[28] J. C. Rimada, L. Hernandez, K. W. J. Barnham, J. P. Connolly, Quantum and conversion efficiencies calculation of AlGaAs/GaAs multiple quantum well solar cells, Phys. Status Solidi B 242 (9) (2005) 1842-1845.

[29] J. C. Rimada, L. Hernandez, J. P. Connolly,K. W. J. Barnham, Conversion efficiency enhancement of AlGaAs quantum well solar cells,Microelectron. J. 38 (2007) 513-518.