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Monte Carlo Model for Carrier Transport in Quantum Well Solar Cell

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ABSTRACT

In this paper, a Monte Carlo model for electron and hole transport in GaAs/AlGaAs quantum well solar cells (QWSCs) is presented. In the model, the quantum mechanical limitations of particles are considered. By appropriate combination of the classical and quantum equations the tunneling behavior, quantization of energy levels, quantum reflection of carriers, and some other properties of the QWSCs have been modeled. Especially, the model is able to calculate the dark and optical currents, simultaneously. The accuracy of the model is compared with published practical results. Graphic energy diagram of particles is a unique trait of this model that is earned at last. Modeling is based on the ensemble Monte Carlo method (EMC). The simulations were achieved using the MATLAB software.
KEYWORDS: Monte Carlo, Quantum Well Solar Cell, Tunneling, Reflection, Transition, Wave function, Super particles.

1. INTRODUCTION

Quantum Well Solar Cells (QWSCs) have been widely used in satellites and modern wireless systems[1], [2] and [3].Introducing quantum wells (QW) into the intrinsic region of the solar cell, results in a better conversion efficiency compared with the conventional p-i-n solar cells[4] and [5].Such configuration has two main advantages in which the absorption of low energy photons in the shallow wells leads to the increase in the short circuit current and open circuit voltage, since the recombination rate increases in the wells[6].The well width and the Al mole fraction of GaAs/AlGaAs cells play significant roles in the capture and escape of carriers and the efficiency of the cells [6].The highest efficiency reported for this type of cells, used in the satellites, is 41.6% fora triple junction InGaP/InGaAs/Gesolar cell [1].

Despite a large amount of researches achieved so far on the solar cells, a few works have been focused on the QWSCs[7].In 1993 Corkish and Green developed a model for QWSC in which the quantum well was a separate cell in parallel with the main cell[8].Separation of the QW from the main cell does not show appreciable effects on the cell efficiency compared with the traditional cells, but it was useful to show various absorption and recombination effects in traditional cells. Mohaidat proposed another model in 1994, where the tunneling of the carriers in multi-quantum wells was considered [9].Based on this model, it was possible to show that the efficiency will increase significantly, if the tunneling rate of the carriers is made optimum. In a model proposed by Varonides, having good agreement with the experimental results, the effect thermal distribution on the cell was considered and its effect on the total carrier concentrations and the tunneling phenomena were analyzed simultaneously[10],[11]. In 2008 a model was presented in order to study the effect of escape and capture phenomena in QWSC [12].Each of the aforementioned models had focused on just on property of the QW. The model proposed in the present work will be able to analyze all properties of the QWSC. Such a comprehensive model requires the consideration of the actual behavior of the quantum particles, electrons and holes. Some models like Drift-Diffusion and hydrodynamic models are suitable for large scale devices, but in QWs, some phenomena like saturation of the velocities in high electric fields and the thermal velocity will add some unpredictable errors into the results. Some works have been achieved to overcome these problems [13],[14] and [15].But these proposed solutions have usually led to the models that are still unable to predict new phenomena. The Monte Carlo method used in this work can give precise results by considering every equation for particle behavior.

The aim of this paper is to prepare a Monte Carlo model for a single QWSC. The method has a significant difference with the above mentioned and the other methods, since it is directly based on the physical and mathematical aspects of the particle behavior and no assumption needs to be made in the model. Any physical phenomenon happened in the real world, can be modeled by the Monte Carlo method. Thus, the more the physical equations are included in the model, the more the accurate results [16].

The scientific contributions of this paper are: 1) solving the Poisson equation with the transferred matrix method (TMM), 2) calculation of the energy eigenvalues and the wave functions in each mesh, 3) Monte Carlo modeling of

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the tunneling process by calculation of the tunneling probability, 4) Modeling of reflection and transition phenomena of particles at the material boundaries.

II. Quantum Well Solar Cell and Monte Carlo model

Monte Carlo methods use randomly generated numbers or events to simulate random processes and estimate complicated results. Particles transportation in semiconductor devices is a random phenomenon. So, this method can be applied to model the carrier transportation. The Monte Carlo method used in this paper is described in [17] and [18]in detail, where the equations regarding scattering, drift, Poisson and Monte Carlo simulation of such phenomena are included.

In this work we have used the Monte Carlo method for a special solar cell in which a quantum well is included, and the limitations added to the classical Monte Carlo method for this structure will be tackled.

A sample quantum well solar cell used in this work and its energy bands are shown in

Fig.1,where the middle layer forms a quantum well.

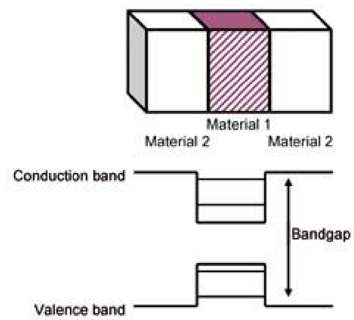


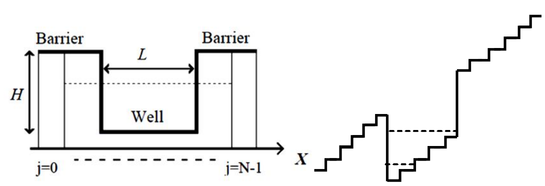
Fig.1. A sample quantum well junction

At first, the tunneling and the energy of carriers are considered. The energy of carriers in the well is calculated by solving the Schrödinger equation:

$$\left[\frac{-h^2}{8\pi^2}\frac{d}{dx}\frac{1}{m(x)}\frac{d}{dx}+V(x)\right]\psi(x)=E\psi(x) \qquad (1)$$

Where$h$ is thePlank constant, m is the effective mass of electron, V is the electrostatic potential,ψ is the wave function of electron, and E is the energy of the particle.

Since the Monte Carlo method needs to divide the device into smaller meshes, the Schrödinger equation has to be discretized to solve. The meshes used in this work are equal in size. Therefore, the Schrödinger equation will be solved using the Transfer Matrix Method (TMM) [19].The potential has a special value in each mesh.



(a) (b)

Fig.2.Potential profile in Quantum well a) non field b) in the presence of field.

The equations used in the TMM method to solve the 1-D Schrödinger equation are listed below:

$$\psi_j(x)=A_j e^{p_j(x)}+B_j e^{-p_j(x)} \qquad (2)$$

$$p_j(x) = \begin{cases} \Gamma_0 x & j = 0 \\ \Gamma_j (x - x_{j-1}) & j > 0 \end{cases} \tag{3}$$

$$\Gamma_j(E) = i\sqrt{\frac{8\pi^2 m_j}{h^2}(E - V_j)} \tag{4}$$

Where A_j and $B_j$are determined by the boundary conditions. j is the integer index of the layers varied between 1 to N (the number of meshes). By considering the continuity condition of the wave function and its derivative at the boundaries of the layers, will results in

$$\begin{bmatrix} A_{j+1} \\ B_{j+1} \end{bmatrix} = M_j \begin{bmatrix} A_j \\ B_j \end{bmatrix} \tag{5}$$

By multiplying M_j's to each other:

$$\begin{bmatrix} A_{N-1} \\ B_{N-1} \end{bmatrix} = \begin{bmatrix} \alpha_{11} & \alpha_{12} \\ \alpha_{21} & \alpha_{22} \end{bmatrix} \begin{bmatrix} A_0 \\ B0 \end{bmatrix} \tag{6}$$

Considering the limitations of A_j and $B_j$at$j$=0 and j=N, it is found that α_{22} must be zero (α_{22} =0). Therefore, any particle energy E that satisfies this condition is one answer to the Schrödinger equation.

According to these relations the energy of carriers will be calculated. In Table 1the energy levels obtained for the well-used in this work (GaAs/AlGaAs, width=100Å, height=0.374eV for electrons and 0.187eV for holes) are summarized. The height of the well for the holes is small. Therefore, the holes can get only one level of energy in the well. Wave functions will be obtained by a recursive method using equations (2)-(4) and the energies listed in Table 1.The resulting wave functions in the sample QWSC are shown in Fig.3 for electrons:

Table 1. The energy of carriers with TMM method in sample QWSC

Energy	Hole	Electron
E1	0.11805	0.0549
E2	-----------	0.1552
E3	-----------	0.3115

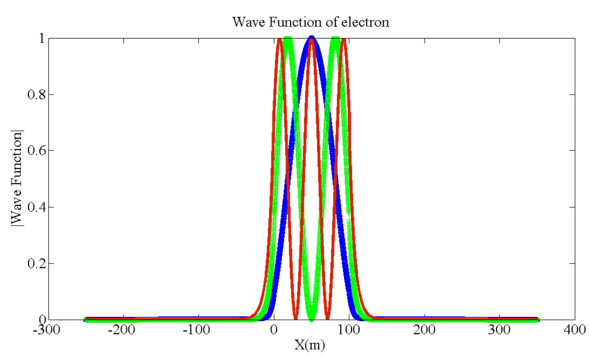


Fig.3. Wave function of electrons for the sample cell for E1 (blue), E2 (green) and E3(red).

The wave functionis a measure of existing probability of a particle. Therefore, if the wave function extends to the edges of the potential walls, the relevant particle can tunnel through the barrier(Fig.4). Fig.3implies that indeed the electrons can tunnel through the barriers, because their wave functions have non-zero values beyond the 100Å well. Electrons in the well have quantized energy levels. The higher the energy level, the larger the probability of tunneling.

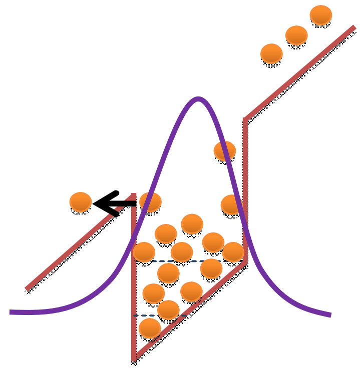


Fig.4. Carriers tunneling from quantum well

Equation 7represents the tunneling probability as a function of wave function [20]:

$$T = \frac{|\psi(x_j)|^2}{|\psi(x_{j-1})|^2} \tag{7}$$

Therefore, the probability of tunneling from the layer*j*into the layer*k* is:

$$TUN = \frac{|\psi(x_{j-k})|^2}{|\psi(x_j)|^2}, \quad k = 1,2,\ldots,N \tag{8}$$

According to equation (8), the carriers can tunnel from the left to the right of the well inFig.4for which $\psi(x_{j-k})$ is non-zero. For use in the Monte Carlo simulation, *TUN* has been normalized in Fig.5.

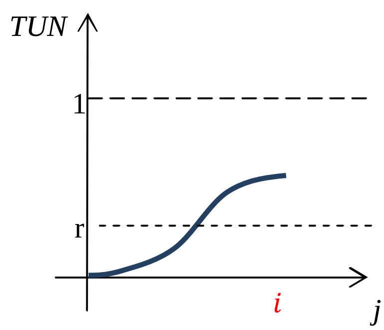


Fig.5. Tunneling probability into the *i*layer from other layers.

Now, referring to the above equations, the tunneling phenomenon can be implemented using the Monte Carlo random generation method:

$$\begin{cases} r < Tun & \text{Tunneling} \\ r > Tun & \text{Reflection} \end{cases}$$

Another important phenomenon needs to be discussed is the reflection of the particles atthe material boundaries, which is a function of the refractive indices of materials[17]. The two parameters describing this property are the reflectivity R and the transition factor T, where

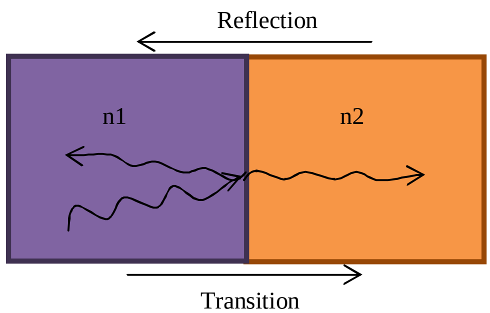


Fig.6. Reflection process form material boundary

$$R = \left(\frac{n1 - n2}{n1 + n2}\right)^2 \quad (9)$$

$$T = \sqrt{1 - R^2} \quad (10)$$

where n1 and n2 are the refractive indices of the two materials. n1 and n2 are functions of wavelength, therefore, the transition rate depends on the wavelength of the incident light.

This phenomenon is implemented in the Monte Carlo method by random generation ofthe numbers, r, as following:

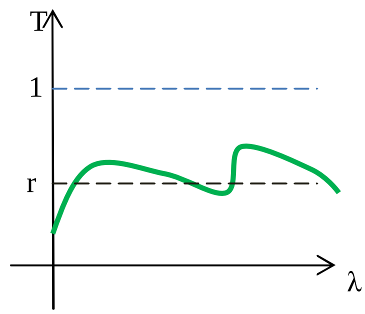


Fig.7. Transition rate versus wavelength.

Where

$$\begin{cases} r<T & \text{Transition} \\ r>T & \text{Reflection} \end{cases}$$

In a solar cell the generation and recombination must also be considered. In our QWSC sample, the doping concentrations of the *n* and *p* regions are about 10^{18}cm^{-3}. In this work it was assumed that there exist 100 super particles [17]in a unit of volume, meaning that each super particle serves as 10^{16}physical particles. Optical generation can significantly increase the minority carrier concentration, while the concentration of the majority carriers remains approximately unaltered. The concentration of the optically generated carriers is about 10^4 to 10^5 cm^{-3}. In this case the defined super particles cannot distinguish the optical carriers, and it will be assumed zero in the simulations. To solve this problem, two types of super particle are assumed; one for the optical carriers and the other for the normal carriers.

Another problem is the recombination lifetime of the carriers. Recombination of carriers takes place in about 10^{-6}s, while the transport time of carriers in a mean free path is in the range of 10^{-12}s. It means that the program needs about 10^6 repeats of the Monte Carlo loop to reach the first recombination. In order to solve this problem, the number of carriers in each cell is determined in steady state.

The first stage of the program requires the appropriate selection of the initial conditions of the carrier properties at thermal equilibrium and in the no-field condition. In each run of the Monte Carlo loop [17] the particles drift and also scatter in the field. In the drift subroutine the tunneling and reflection of carriers are considered.

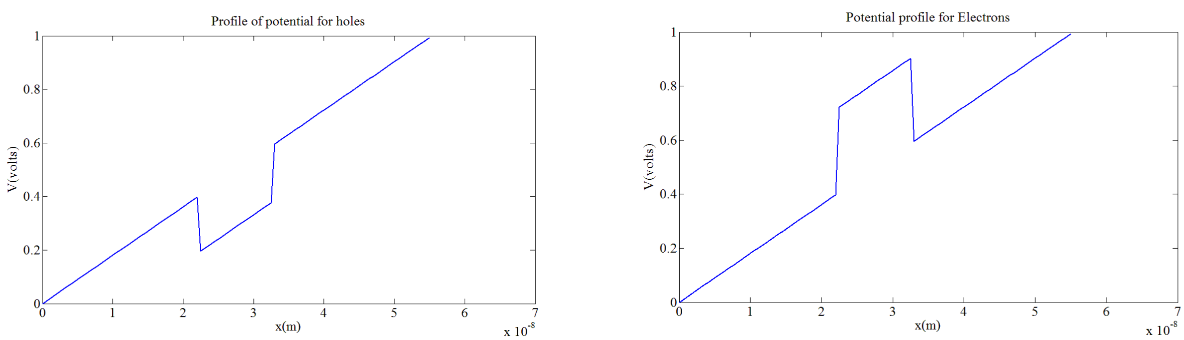
Generation and recombination of the carriers are considered in a subroutine that updates the number of particles in each cell.

Scattering types considered in the QWSC are impurity scattering, phonon scattering and carrier-carrier scattering. In the intrinsic region impurity scattering is not considered. Because of the strong field, the bands are non-parabolic [17].

III. SIMULATION AND RESULT

The program has been run for 500 repeat, Δx=5Å, ΔT=2 fs, Temperature=300°k, concentration of the n and p regions= $2\times10^{18}cm^{-3}$, and the solar spectrum was AM1.5 [21].The well height was calculated to be 0.374eV for electrons and 0.187eV for holes for the mole fraction of x=0.45. The well width was assumed to be 100Å. The results of simulations are discussed below.

The potential profile will be updated after every run of the Monte Carlo loop. The final results are shown in Fig.8.



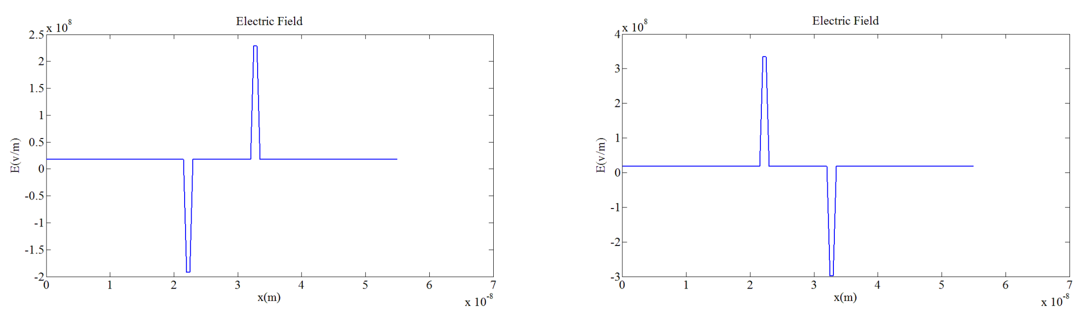
(a) (b)

Fig.8. Potential profiles for a) electron and b) holes.

The size of the device is very small; therefore, the electric field extends to the doped regions.

The electric field is calculated from equation (11):

$$Field = -\frac{V}{\Delta x} \qquad (11)$$

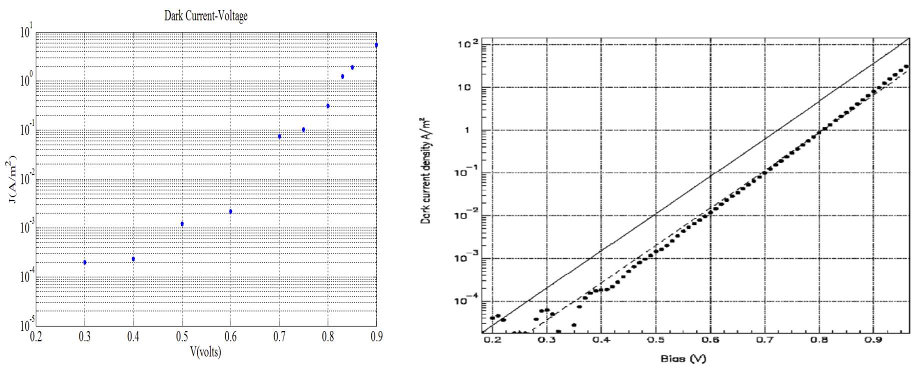


(a)(b)

Fig.9. Field for a) electrons and b) holes.

Negative value of the field shows the barriers against carrier's motion.

Fig.**10**compared the experimental result given in[22]with the current-voltage characteristics obtained from our model with linear approximation for 30 wells. It shows good agreement with experimental result.



(a)(b)

Fig.10 . Comparison of the results obtained from the present work (a) with the experimental result in ref. [22] (b).

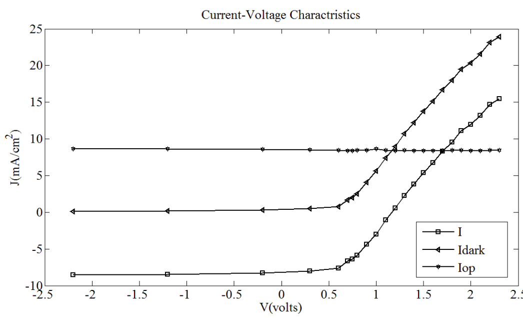
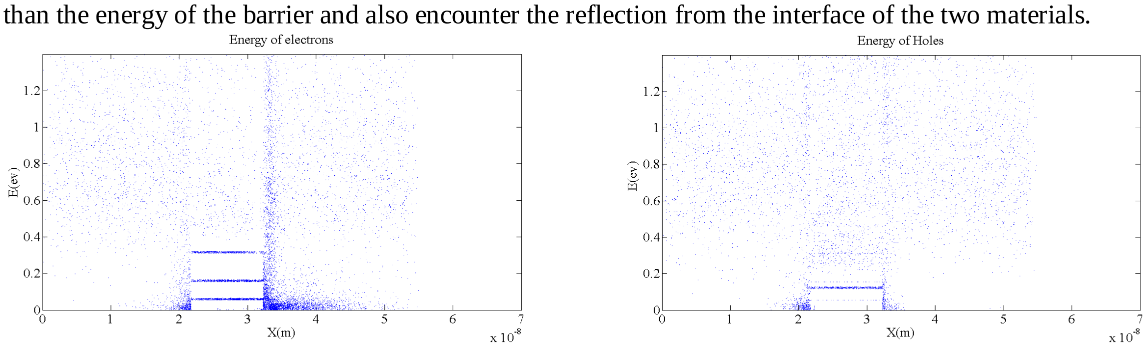


Fig.11. Current voltage characteristics for the sample cell.

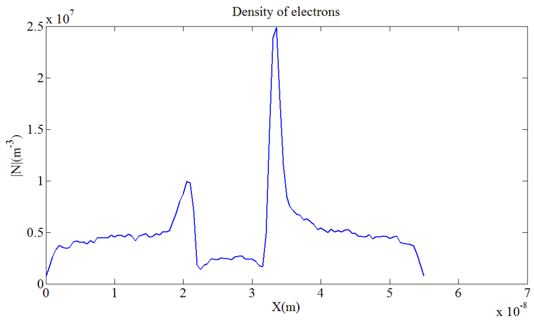
The current-voltage characteristics of the cell are shown in theFig.12.As it is observed the dark and optical currents are shown separately, which is an advantage of the Monte Carlo process, since this model benefits a particle based method of simulation. On the other hand, the energy of the particles can give good information about the recombination and absorption of wavelength spectrum. Fig.12the particles energy in the well is quantized. As can be seen, some carriers surpass the potential wall. Some other carries are confined in the well because their energies are less than the energy of the barrier and also encounter the reflection from the interface of the two materials.

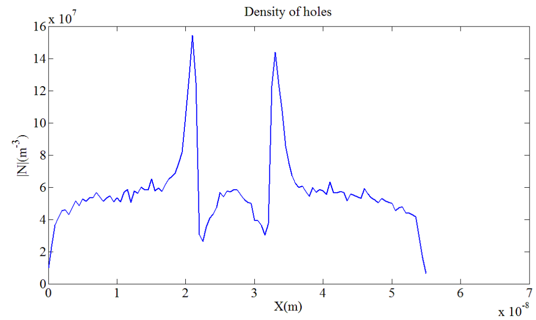


(a) (b)

Fig.12.Particles energy a) electrons b) holes.

The concentration profiles of electrons and holes are shown in Fig.13 According to this figure there is a peak at each interface of the wall, indicating the higher concentration of the carries at the interfaces. These are due to the reflection and capture of the carries at these boundaries. At the contacts, since the carriers are swept out very quickly, the concentrations of carriers are very low.





(a)(b)

Fig.13 concentration profile a) electrons b) holes.

IV. CONCLUSION

A Monte Carlo model for carrier transport is presented in this paper. Particle based analysis is one of the advantages of the Monte Carlo method that makes possible analyze every phenomena such as generation and recombination, tunneling, thermal escape, and capture in the well. This model is also capable of investigating other particle-based phenomena that cannot be analyzed using traditional methods. Using the obtained results it is possible to ultimately obtain the efficiency of QWSCs. At high fields the particle velocity will approach the saturation velocity. Drift-Diffusion and Hydrodynamic equations cannot properly track this velocity. The electric field in a well of 100Å width is several thousand times larger than the field in the bulk. The only method that can simulate the particle transportation in such high fields is the Monte Carlo method. The energies of the particles have also been obtained in detail which can give valuable information regarding the recombination and absorption of wavelength spectrum. The dark and optical currents obtained separately which is an advantage of the proposed model. It is shown that there are good agreement between our results and the experimental results reported in the other works.

The more physics is added to this model, the more accurate results are obtained.

The model presented in this work is a semi-classical Monte Carlo model, because it considers the classical relations of the carrier transport in the bulk AlGaAs and the quantum transport in the quantum well.

REFERENCES

[1] J. G. J. Adams, B. C. Browne1y, I. M. Ballard2, J. P. Connolly3, N. L. A. Chan1, A. Ioannides1, W. Elder1, P. N. Stavrinou1, K. W. J. Barnham and N. J. Ekins-Daukes."Recent results for single-junction and tandem quantum well solar cells", Published online in Wiley Online Library (wileyonlinelibrary.com). DOI: 10.1002/pip.1069. Prog.Photovolt: Res. Appl. (2011).

[2]Lumpp, J.K.; Lumpp, J.E.; Erb, D.M.; Torabi, N.M.; , "The evaluation of solder and circuit board materials for small satellite solar cell arrays," *Aerospace Conference, 2010 IEEE* , vol., no., pp.1-6, 6-13 March 2010doi: 10.1109/AERO.2010.5446720.

[3] Bao Hoang; Wong, F.K.; Corey, R.L.; Gardiner, G.; Funderburk, V.V.; Gahart, R.L.; Wright, K.H.; Schneider, T.A.; Vaughn, J.A.; , "Combined Space Environmental Exposure Test of Multijunction GaAs/Ge Solar Array Coupons," *Plasma Science, IEEE Transactions on* , vol.40, no.2, pp.324-333, Feb. 2012doi: 10.1109/TPS.2011.2174161.

[4] K.W.J. Barnham, "A novel approach to higher efficiency-the quantum well solar cell", 11th E.C. Photovoltaic Solar Energy Conference, Montreux, Switzerland, pp. 146–149, 1992.

[5] A. Ibrahim," LBIC Measurements Scan as a Diagnostic Tool for Silicon Solar Cell", Journal of Basic and AppliedScientific Research, ISSN 2090-424X, 2010.

[6] Stephen M. Ramey and Rahim Khoie, "Modeling of Multiple-Quantum Well Solar Cells Including Capture, Escape, and Recombination of Photoexcited Carriers in Quantum Wells", IEEE TRANSACTIONS ON ELECTRON DEVICES, VOL. 50, NO. 5, MAY 2003.

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

[8] R. Corkish, M. Green, “Recombination of carriers in quantum well solar cells”,Proceedings of the 23rd Photovoltaic Specialists Conference, Louisville, 1993, p. 675.

[9] J.M. Mohaidat, K. Shum, W.B. Wang, R.R. Alfano,” Barrier potential design criteria in multiple-quantum-well-based solar-cell structures” J. Appl. Phys. 76 (1994) 5533.

[10] Varonides A.C, & etc,“1 cm×1 cm GaAs/AlGaAs MQW solar cells under one sun and concentrated sunlight” Proceedings of the Second World Conference on Photovoltaic Solar Energy Conversion, Vienna, 1999, p. 66.

[11]A. Varonides, “Thermionic escape of net photo generated carriers and current densities from illuminated lightly doped single quantum wells”, Physica E 14 (2002) 142.

[12]Chin-Yi Tsai; Chin-Yao Tsai; , "Effects of carrier escape and capture processes on quantum well solar cells," *Numerical Simulation of Optoelectronic Devices, 2008. NUSOD '08. International Conference on* , vol., no., pp.79-80, 1-4 Sept. 2008doi: 10.1109/NUSOD.2008.4668251.

[13]Carlo de Falco, Emilio Gatti, Andrea L. Lacaita, Riccardo Sacco,” Quantum-corrected drift-diffusion models for transport in semiconductor devices”, Journal of Computational Physics,Volume 204, Issue 2, 10 April 2005, Pages 533–561.

[14] Fardi, H.Z.; , "Numerical modeling of hot electron GaAs/AlxGa1−xAs quantum well photovoltaic," *Photovoltaic Specialists Conference (PVSC), 2010 35th IEEE* , vol., no., pp.001800-001803, 20-25 June 2010 doi: 10.1109/PVSC.2010.5615914.

[15] F. Haas, G. Manfredi, P. K. Shukla, “Breather mode in the many-electron dynamics of semiconductor quantum wells”, The American Physical Society journal, DOI: 10.1103/PhysRevB.80.073301, published 14 August 2009.

[16] C. Moglestue, “Monte carlo simulation of semi counductor device”, Chapman & Hall, 1993.

[17] Kazutaka Tomizawa, “Numerical Simulation of Submicron Semiconductor Device”, Artech House, ISBN 0-89006-620-5, 1993.

[18]CarloJacoboni and Lino Reggiani,” *The Monte Carlo method for the solution of charge transport in semiconductors with applications to covalent materials*”, Rev. Mod. Phys ..Vol. 55.No.3. July 1983.

[19]B. Jonsson, Sverre T. ENG, “Solving the Schrodinger Equation in Arbitrary Quantum-Well Potential Profiles Using the Transfer Matrix Method”, IEEE journal OF Quantum Electronics, vol. 26, no. 11, November 1990.

[20] Kwok K. Ng, Complete Guide to Semiconductor Devices, 2nd Edition, ISBN: 978-0-471-20240-0, July 2002, Wiley-IEEE Press.

[21] S. M. Sze, Kwok K. Ng, “Physics of Semiconductor Devices”, 3nd Edition, ISBN-13: 978-0-471-14323-9,2007,New Jersey, Wiley.

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