NUMERICAL SIMULATION OF MULTI-QUANTUM WELL SOLAR CELLS GAAS / ALGAAS

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ABSTRACT

Inserting Multi-quantum well into solar cells proved to be a promising technique for producing high efficiency third generation solar cells. The presence of quantum well increases the absorption spectra into longer wavelengths, therefore increasing the short-circuit current density while maintaining the open-circuit voltage at acceptable level [2;3]. In this work;we evaluate the generated photocurrent in an $Al_xGa_{1-x}As/GaAs$ *p-i-n* solar cell using a simple approach. Firstly Schrödinger equation is solved numerically to determine the confined energy states in a single quantum well; the second step consists of calculating the absorption coefficient $\alpha(\lambda)$ taking into account the allowed valence to conduction bands transitions. Finally the total photocurrent is analysed for various structure parameters specifically; width, height (related to the Aluminum concentration x), and number of wells inside the intrinsic layer. The simulated results confirm the enhancement brought about by the presence of quantum wells.

Key Words: *solar cell, quantum well, absorption coefficient.*

1. INTRODUCTION

The quantum well solar cell (QWSC) was first introduced by Barnham and co-workers [1] as a novel device in which a series of quantum wells (QWs) forms the *i*-layer of a *p-i-n* solar cell. Studies have shown that the insertion of such a series of quantum wells into the depletion region of a solar cell can significantly enhance the cell's short-circuit current and hence the efficiency of the solar cell [2, 3]. Higher photocurrent can be generated if wells are deeper, since longer wavelengths are then absorbed [4]. The incorporation of the multiple quantum wells (MQWs) has two counteracting effects: the short-circuit current is increased because of the additional absorption of low-energy photons in the lower band-gap quantum wells; and the open-circuit voltage is decreased because of the increased recombination of carriers trapped in the quantum wells [5]. The photocurrent is then determined by lower-band-gap (well) material, while the output voltage would be determined by barrier material. The characteristics of the well, its width and depth, determine the absorption edge and the spectral response of the MQW solar cell. Longer wavelengths can be absorbed if the quantum well is deeper, leading to a higher photocurrent in the cell. Whereas, the output voltage is related to the width of the host material band gap, the recombination in the well and interfaces between barriers and wells. Therefore, in choosing the depth of the wells one has to compromise between the photocurrent and the output voltage. The number of wells is an important factor too, wider wells improve the absorption, but a smaller number of wells fit in the intrinsic region. Whereas, a large number of narrow wells with lower photon absorption can be inserted in the same intrinsic layer. Increasing the number of wells enhances the photocurrent provided the recombination at the interfaces is reduced.

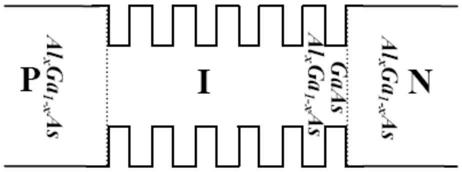


Fig. 1. Schematic diagram of the investigated *p-i-n* $Al_xGa_{1-x}As$/ GaAs MQW/ $Al_xGa_{1-x}As$ solar cell. Layers parameters respectively are: ***P***; 0.05 µm, $p = 10^{19}cm^{-3}$, ***I***; 1µm, $n = p = 1.79 \times 10^{6}cm^{-3}$, ***N***; 1µm, $n = 10^{19}cm^{-3}$

2.1 ABSORPTION COEFFICIENT

The calculation of the absorption coefficients of $Al_xGa_{1-x}As$ MQW Schrödinger equation for one dimensional single square quantum well is numerically solved. The quantum-mechanical motion of a carrier inside the well is described by a wave function $\psi_{e,h}(z)$ solution of the Schrödinger equation for the unperturbed potential for electrons *(e)* and holes *(h*) as follows:

$$\left[-\frac{\hbar^2}{2m_{e,h}^*}\frac{d^2}{dz^2}+V_{e,h}(z)\right]\psi_{e,h}(z)=E_{e,h}\psi_{e,h}(z) \qquad 01$$

Where $\hbar$ is Planck constant, $m_{e,h}^*$ is the carrier effective mass, $E_{e,h}$, the carrier energy and $V_{e,h}(z)$ is the potential energy of the finite well determined by the energy discontinuity between well and barrier material [5].

In the GaAs /AlGaAs system, this discontinuity can be expressed as *1.247 x* at *T = 300 K* for *x < 0.45*, where *x* represents the mole fraction of the Aluminum in the alloy. The finite difference technique is used for the solution of the Schrödinger equation mainly due to its simplicity and efficiency for this kind of problems[6;7].The well absorption coefficient is then calculated by summing over the electron-heavy hole and electron-light hole transitions:

$$\alpha_w(E)=\alpha_c(E)+\sum_n \alpha_{e_n-hh_n}(E)+\sum_n \alpha_{e_n-lh_n}(E) \qquad 02$$

Where $\alpha_c(E)$ is the absorption coefficient of the continuum:

$$\alpha_c(E)=A\left(h\nu-E_g\right)^{1/2} \qquad 03$$

Where $A = 3.5.10^4$ cm^{-1} (for $Al_xGa_{1-x}As$ for $x < 0.4$), and $E_g(x) = 1.424$ eV + x 1.247 eV [8]. $\alpha_{e_n-hh_n}(E)$ and $\alpha_{e_n-lh_n}(E)$ are the well absorption coefficients of the confined *n*th heavy and light holes transitions respectively.

To calculate these parameters we adopt the ideal quantum well model suggested by Rimada and revised later by Lade et al [7]:

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

$$\alpha_{e_n-hh_n}(E)=\frac{\pi q^2 (E_p/3)}{4\pi\varepsilon_0 n_r c m_0 E \ell \hbar}\frac{m_{e,w_{xy}} m_{lh,w_{xy}}}{m_{e,w_{xy}}+m_{lh,w_{xy}}}Y(E-E_n) \qquad 4.b$$

where Y is the step function and ℓ is the quantum thickness of the heterostructure, where $E_P = 23$ eV;, $m_{e,w}$ and $m_{hh,w}$, are the well electron and heavy hole effective masses, ε_0 is the dielectric constant, n_r is the well refractive index, E_n are the transition energies, q the electronic charge, c the speed of light in a vacuum, $\hbar$ is the Planck constant m_0 is the free electron mass. For the electron-light hole transitions E_P is replaced by $E_P/3$ and the heavy hole masse by the light hole masse $m_{lh,w}$ Eq. (4*b*).Figure 2 represents the calculated absorption coefficient $\alpha(E)$ versus the photon energy (*E*) for different well widths (50, 100 and 200 Å) for a fixed aluminium molar fraction $x = 0.4$ ($E_g = 1.922$ eV) in the barrier. The absorption coefficient of the continuum is plotted for comparison. It can be seen clearly that the absorption inside the quantum well is significant, which can be explained simply by the lower confined energy levels inside the well and a shift of the absorption energy threshold towards lower energies. Two distinct regions can be observed; the first one is due to the transition from the bound states in the well and corresponds to low energies. This fraction of the curve has a stair-like shape which fits well with discrete transition levels in both the valence and conduction bands. The number of stairs depends on the number of allowed transitions. The second part of the curve matches with the absorption by the continuum. In figure 3, the absorption coefficient is plotted versus photon energy for different aluminium fraction *x* in the barrier material (0.2, 0.3 and 0.4) while maintaining the well width at 100 Å. The absorption coefficient of GaAs ($x = 0$) is plotted for comparison. The curves comprise of two distinct regions the first one (stair-like form) illustrates the contribution of the bound states in the well while the second represents the absorption of the continuum energy range. As the fraction *x* is increased the depth of the well is increased then absorption threshold shifts to greater energies and the number of stairs is also increased.

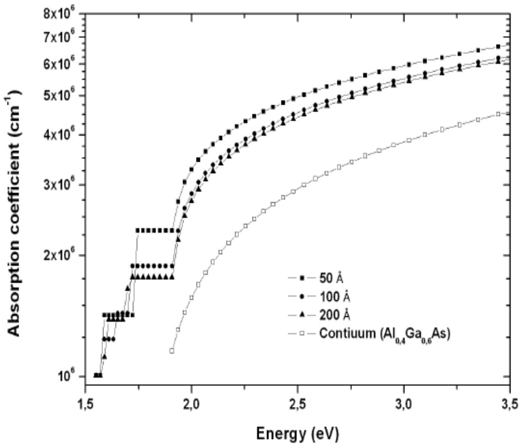


Fig. 2. Absorption coefficient of a $Al_{0.4}Ga_{0.6}As/GaAs/Al_{0.4}Ga_{0.6}As$ single quantum well for different thicknesses

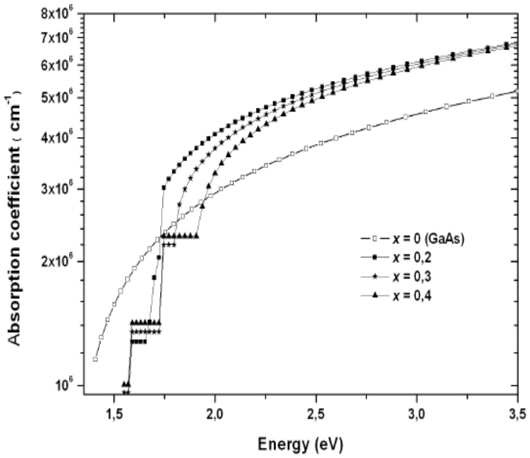


Fig. 3. Absorption coefficient of a $Al_xGa_{1-x}As/GaAs/ Al_xGa_{1-x}As$ 100 Å single quantum well for different aluminium molar fractions *x*.

2.2. SPECTRAL RESPONSE

The total photocurrent generated by the quantum well solar cell is the sum of the photogenerated current at the *n* and *p* layers together with current at the intrinsic layer[9].

$$J_{ph}(\lambda) = J_{Ph,n}(\lambda) + J_{Ph,p}(\lambda) + J_{ph,IQW}(\lambda) \qquad 05$$

The spectral response is defined as:

$$SR(\lambda)=\frac{J_{Ph}(\lambda)}{qF(\lambda)\left[1-R(\lambda)\right]} \qquad 06$$

Where $F(\lambda)$ is the number of incident photon $/cm^2/s$ per bandwidth, and $R(\lambda)$ the fraction of these photons reflected from the surface. The analysis is carried out under one AM1.5. Empirical expression approximating photon flux density $F(\lambda)$ is adopted from Ref. [10]. Figure 4 shows the spectral response of $Al_{0.4}Ga_{0.6}As$/GaAs MQW/$Al_{0.4}Ga_{0.6}As$ solar cell with 20 wells for different well widths respectively 50, 100 and 200 Å. From this figure we can see that for greater wavelengths $(\lambda > 0.6\mu m)$ the spectral response improvement is significant, particularly for wider wells. This is attributed to the absorption of photons with longer wavelengths. In this region of the spectre the *SR* has a stair-like shape this is because of the wells absorption coefficient, as discussed above. Whereas for wavelengths between 0.2μm and 0.6 μm there is a slight improvement as the wells width is increased. The limitation of the wells number is due to restriction of the intrinsic layer thickness, which is limited to 1 μm in this work.The effect of the number of wells (10 to 30 wells) on the spectral response of $Al_{0.4}Ga_{0.6}As$/GaAs MQW/ $Al_{0.4}Ga_{0.6}As$ solar cell is shown in figure 5; the wells are 100 Å wide.

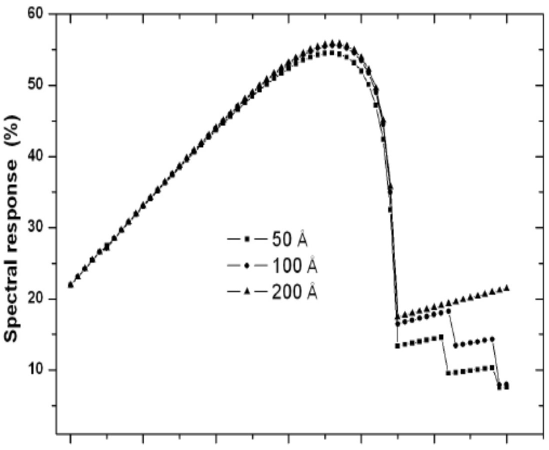
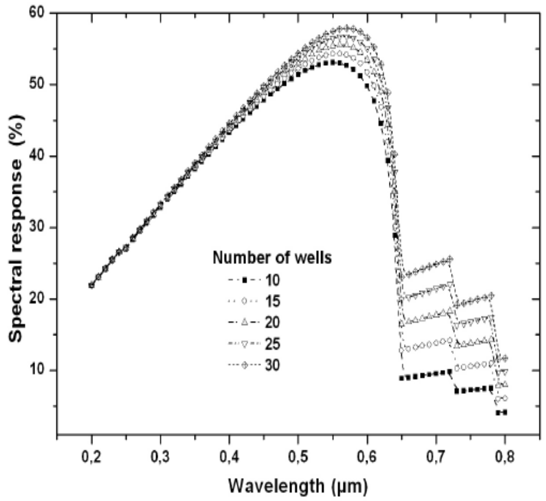


Fig. 4. Internal spectral response SR (λ) of $Al_{0.4}Ga_{0.6}As$/GaAs MQW /$Al_{0.4}Ga_{0.6}As$ solar cell with 20 wells for different thicknesses.



$Al_{0.4}Ga_{0.6}As$ solar cell with 100 Å wide wells for different well numbers.

The improvement of the *SR* is remarkable, particularly for longer wavelengths (λ >0.6 μm). This could be explained by the absorption of an increased numbers of photons with longer wavelengths. The increase of the wells number has the tendency of widening the part of semiconductor (*GaAs*) having smaller energy band gap (*1.424 eV*), thus more 'longer wavelengths' photons are absorbed. This situation is very similar to the case of double junction tandem solar cell with $E_{g1} = E_{g,\mathrm{AlGaAs}}$ and $E_{g2} = E_{g,\mathrm{GaAs}}$. We can deduce from the dependency of the internal spectral response on the width and the number of wells in the intrinsic layer of an $Al_xGa_{1-x}As$/GaAs MQW/ $Al_xGa_{1-x}As$ solar cell that the best cell should have as many as possible wider wells. Unfortunately, there are many technological and physical factors that act against this, therefore a compromise is needed. The main limit is the size of the intrinsic layer which could not be much thicker, to maintain the uniform electric field and ensure an even absorption. On the other hand, increasing the number of wells will augment the number of interfaces leading to a growing recombination.

3. Photocurrent Density

Figure 6 shows the total photocurrent of $Al_{0.4}Ga_{0.6}As$/GaAs MQW/$Al_{0.4}Ga_{0.6}As$ solar cell versus the wells thickness for different number of wells. From this graph we can see that the photocurrent generally increases when the numbers of wells is increased, while it has the tendency to saturate if the well thickness is increased. Therefore, the only limit to improve the performance is the maximum number of wells that the intrinsic layer could host. From the conducted investigation we arrived to an optimal configuration of the $Al_{0.4}Ga_{0.6}As$/GaAs MQW/ $Al_{0.4}Ga_{0.6}As$ solar cell, that is; 20 wells of 100 Å in 1µm thick intrinsic layer. The photocurrent of this optimized structure is 29.2 mA/cm^2 compared to 20.5 mA/cm^2 of a single $Al_{0.4}Ga_{0.6}As$ *p-i-n* cell, which represents a gain of more than 40%. To make this type of cells more competitive other aspects has to be analyzed i.e., it is needed to reduce its dark current in order to minimize the reduction of the open circuit voltage therefore improving the energy conversion efficiency.

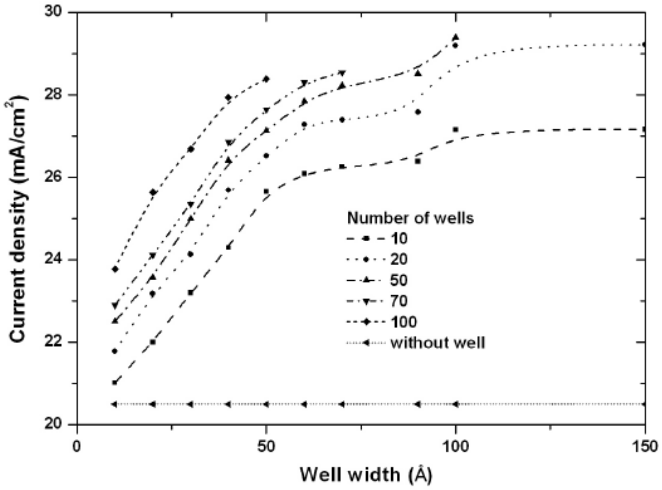


Fig. 6. Total photocurrent of $Al_{0.4}Ga_{0.6}As$/GaAs MQW/ $Al_{0.4}Ga_{0.6}As$ solar cell plotted as function of the wells thickness for different number of wells.

5. Conclusion

There is no doubt that the insertion of quantum wells in a *p.i.n* structure solar cell will improve its short circuit current. In the conducted study we showed that the width in addition to the number of wells has a remarkable effect on the photocurrent of $Al_{0.4}Ga_{0.6}As$/GaAs MQW/ $Al_{0.4}Ga_{0.6}As$ solar cells. Using a simple approach with the previously revised model of Rimada applied to an idealised quantum well, we were able to demonstrate that the photocurrent of a quantum well solar cell will augment with increasing either the width or the number of wells in the intrinsic region. This improvement could be achieved provided that thickness of the intrinsic layer is not over taken. In addition, the thickness of the *i*-layer should not be too thick to avoid the perturbation of the electric field, which is essential for photogenerated carriers' collection. Alternatively, the insertion of a large number of quantum wells (lower band gap) in the *i*-layer is expected to reduce the open circuit voltage, thus it is important to deal with these opposing effects. A complementary work is under way to examine the effect of quantum wells parameters (depth, width and number) on the dark current, open circuit voltage and the energy conversion efficiency.

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