THEORETICAL STUDY OF THE POTENTIAL OF MULTIPLE QUANTUM WELL SOLAR CELLS BASED ON AlxIn1-xAs/GayIn1-yAs

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Improving photovoltaic conversion efficiency requires improving the mechanisms involved in the manufacturing process by making a good choice for the structure of the cell. Today the development of quantum well solar cells has generated great interest. These configurations have shown a good performance. In this work, we investigated the effective potential of multiple quantum well solar cells (MQWSC), from tandem a-AlInAs / GaInAs parameters, where we studied the effect of number of wells and their widths and the depth of the barrier on the effective band gap and on the yield, the results obtained in the simulation show that the potential of this compound III-V to reach a wide range of effective band gap intervals ranging from 2.21 to 0 , 70 eV and the theoretical yield of this type of cells in the theoretical field η = 57.3% for a global AM 1.5 radiation forced in series.

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1. Introduction

The idea of hetero structures has been proposed in order to observe the Bloch oscillations of electrons, and subsequently to obtain microwave generators and amplifiers [1]. It has therefore been suggested to use modulation of alloy composition or doping [2]. Thanks to the growth development, it has become possible to develop super-lattice structures, photonic crystals and quantum wells. Because of these very interesting optical and electronic properties, this latter variety has attracted considerable interest and has been the subject of numerous studies during the last decades. A heterogeneous quantum well structure consists of a material A sandwiched between two barriers of a material B. The quantum denomination occurs when there is confinement of the carriers, that is to say for thicknesses of lower wells typically at 300 Å. Depending on the confinement of carriers, there are different types of quantum structures, the three main configurations are shown in Fig. 1.5:

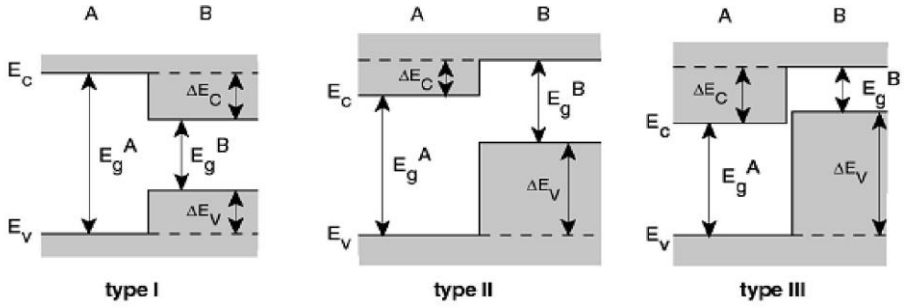

Fig. 1. Schematic diagrams showing three different types of hetero-junction [3].

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The theoretical results, obtained by the authors under an AM1.5 spectrum, show that for a cell with a single junction with a gap of 1.34 eV, a yield of 33.68% and a yield of 45.71% are obtained for a double cell, junction with the gaps 0.94 and 1.60 eV. While for a cell with seven junctions we have the highest efficiency of 60.78% [4]. According to the results obtained by the researchers, it can be confirmed that with a multi-junction cell will obtain a better yield, only the manufacture of this kind of structure remains very limited given its complexity and high cost. Currently a Franco-German team has just developed a solar cell for which they measured a record efficiency of 44.7% [5,6]. They added four junctions to convert the maximum of the solar spectrum energy into electrical energy. In this work, we have theoretically studied a type I hetero structure cell based on the AlxIn01-xAs / GayIn1-yAs semiconductors where the electrons and holes are confined in the well represented by the GayIn1-yAs semiconductor. Last is a key element in active regions of high speed electronic devices. We are talking about a two-dimensional structure, because of deferent well thickness .So can say that the goal of this study is to improve the performance of multiple quantum well solar Cells (MQWSC).

2. Quantum structures

The model chosen for our study is a hetero-junction solar cell based on $Al_xIn_{1-x}As$ / $Ga_yIn_{1-y}As$ alloy, having a type I quantum structure, consisting of the two no doped $Al_xIn_{1-x}As$ and $Ga_yIn_{1-y}As$ semiconductors. This semi-conductor pair makes it possible to create sheltered interfaces and thus to produce fairly complex stacking structures. The quantum well consists of a structure of $Ga_yIn_{1-y}As$, of length Lw, sandwiched between two layers of $Al_xIn_{1-x}As$ of width Ld figure (2). Since the active zone of the structure consists of several wells, it is sufficient to study the properties are the characteristics of these wells.

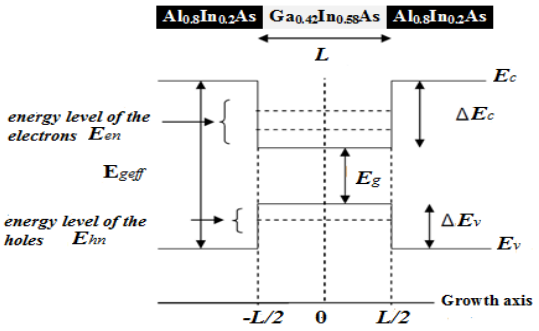

Fig. 2. Energy band diagram in a quantum well ($Al_{0.8}In_{0.2}As$ / $Ga_{0.42}In_{0.58}As$).

3. Theoretical model

The most used formalism for modeling planar hetero-structures is that of the envelope function, in which the variations of the wave functions at the atomic scale are averaged and the states are described by a slowly variable envelope function whose dynamics are governed by effective parameters (effective mass, band shift, etc.). Fig. 2 represents a quantum well, is formed by a thin $Ga_{0.42}In_{0.58}As$ semiconductor layer (well material) placed between two layers of a semiconductor $Al_{0.8}In_{0.2}As$ (barrier material). In the formalism of the envelope function, the Hamiltonian of such a structure is written:

$$H = E_b + V(z) - \frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m_i^*(z)}\frac{\partial}{\partial z} \tag{3.1}$$

Or the band energy E_b is zero for the valence band, and $E_b = E_g$ is the width of the forbidden band of the material $Al_{0.8}In_{0.2}As$, for the conduction band; and $m_i^*(z)$ the effective mass in the growth direction z:

$$m_i^* = \begin{cases} m_{wi}^* \text{ in the material } Ga_{0.42}In_{0.58}As \\ m_{bi}^* \text{ in the material } Al_{0.8}In_{0.2}As \end{cases}$$

V (z) is the potential of the quantum well:

$$V(z) = \begin{cases} V_0 \quad in the material \quad Ga_{0.42}In_{0.58}As \\ 0 \quad in the material \quad Al_{0.8}In_{0.2}As \end{cases}$$

In the quantum well, the potential of the hetero-structure depends only on z, to model the electronic confinement in the quantum wells $Al_{0.8}In_{0.2}As$ / $Ga_{0.42}In_{0.58}As$ / $Al_{0.8}In_{0.2}As$, we will use the approximation of the envelope function and the Schrödinger equation. Take the following form:

$$H\psi = E\psi \tag{3.2}$$

$$\left(E_b + V(z) - \frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m_i^*(z)}\frac{\partial}{\partial z} \right)\psi_i(z) = E_i(z)\psi_i(z) \tag{3.3}$$

$$\left(-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m_{wi}^*(z)}\frac{\partial}{\partial z} \right)\psi_i(z) = E_i(z)\psi_i(z) \tag{3.4}$$

$$\left(E_b + V(z) - \frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m_{b_i}^*(z)}\frac{\partial}{\partial z} \right)\psi_i(z) = E_i(z)\psi_i(z) \tag{3.5}$$

The state of a particle in a semiconductor can be described from the wave function ψ_i (z), which is the solution of the Schrödinger equation ((3.4), (3.5)). Solutions can take the form of plane waves. The effective gap energy between the bound states in the valence and conduction bands will be obtained from:

$$E_{geff} = E_{e_n} + E_{h_n} + E_g \tag{3.6}$$

4. Simulation parameters

The calculation requires input parameters such as effective mass of electrons, light and heavy holes, height of the barrier, width of the well as well as the characteristics of each layer constituting the structure to be simulated. The parameters of $Ga_yIn_{1-y}As$ useful for the calculation are evaluated from a linear interpolation between InAs and GaAs parameters, where we determined the value of the mole fraction y = 0.42 we introduced the rest of the parameters in Table 1. And for the ternary alloy $Al_{0.8}In_{0.2}As$ we fixed the value of the molar fraction x = 0.8, the other parameters are collected in Table 1.

Table 1. Parameters used in the simulation.

	$Al_xIn_{1-x}As$	$Ga_yIn_{1-y}As$
a (A°)	5.677 + 0.501x − 0.080(x^2) [7]	6.05–0.405x[8]
Eg(eV)	0.359 +1.931x +0.720(x^2) [7]	0.359 +0.491y +0.580(y^2) [8]
m_e^*/m_0	0.024 +0.088x +0.012(x^2) [7]	0.024 + 0.034y + 0.0091(y^2) [8]
m_{hl}^*/m_0	0.026+0.134x[7]	0.026 + 0.04y + 0.02(y^2) [8]
m_{hh}^*/m_0	0.024 +0.088x -0.012(x^2) [7]	0.36 + 0.335y–0.145(y^2) [8]

E_g: band-gap, m^*_e/m_0,m^*_{hl}/m_0,m^*_{hh}/m_0: effective masse of electron, light hole and heavy hole respectively.

5. Results and discussion

In this Party we will present the results of the simulations for the quantum well solar cell based on $Al_{0.8}In_{0.2}As$ / $Ga_{0.42}In_{0.58}As$ / $Al_{0.8}In_{0.2}As$. First, we will study the influence of different parameters (quantum well thicknesses (L_w) and quantum barriers (L_b), number of wells (M)) on the energy levels (bound states), which are in the well, the conduction band electrons and the light and heavy holes in the valence band, and the effective gap energy. We have calculated the variation of the energy states as a function of the width of the wells equation (3.3) and (4.3), these computations are made with program MATLAB R2009b. In Fig. 3 and in Fig. 4 respectively we have presented the variation of energy of the conduction band and the variation of energy of the valence band as a function of the width of a well $Ga_{0.42}In_{0.58}As$ barrier. This is done by setting the number of wells (M) and simultaneously varying the well width from 1 to 30 nm and the thickness of the barrier from 1 to 10 nm and the number of wells (M) from (1 - 3 - 5) wells.

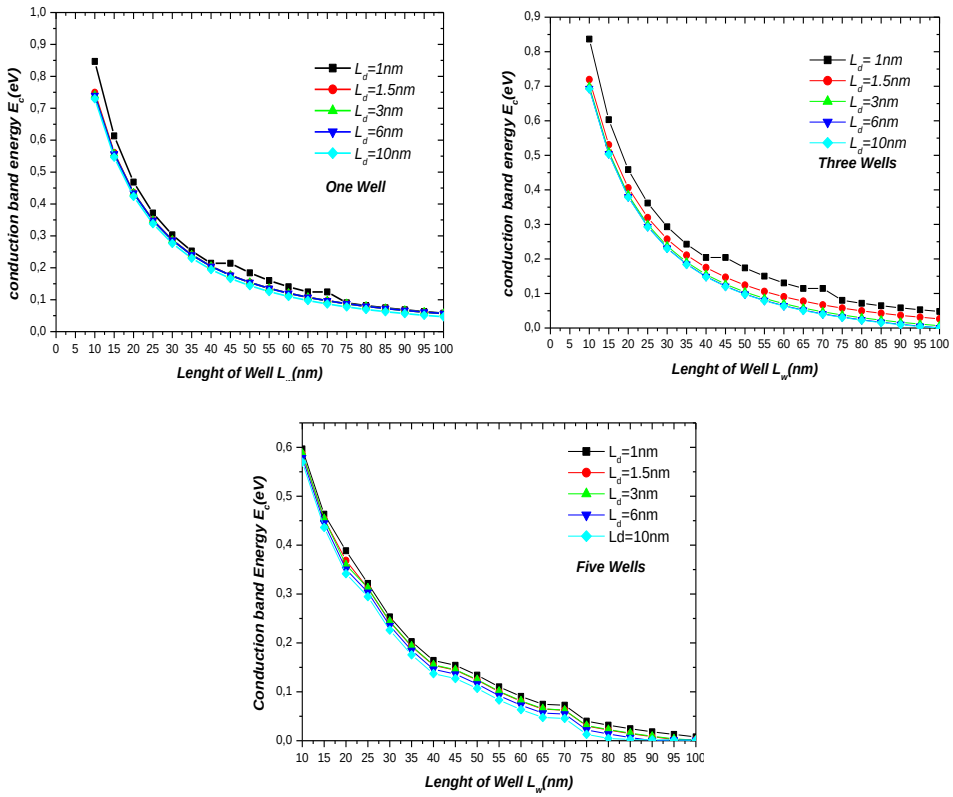

Fig. 3. Conduction band Energy of carriers as a function of the barrier width, the well and the number of the wells for $Al_{0.8}In_{0.2}As$ / $Ga_{0.42}In_{0.58}As$ / $Al_{0.8}In_{0.2}As$ structure.

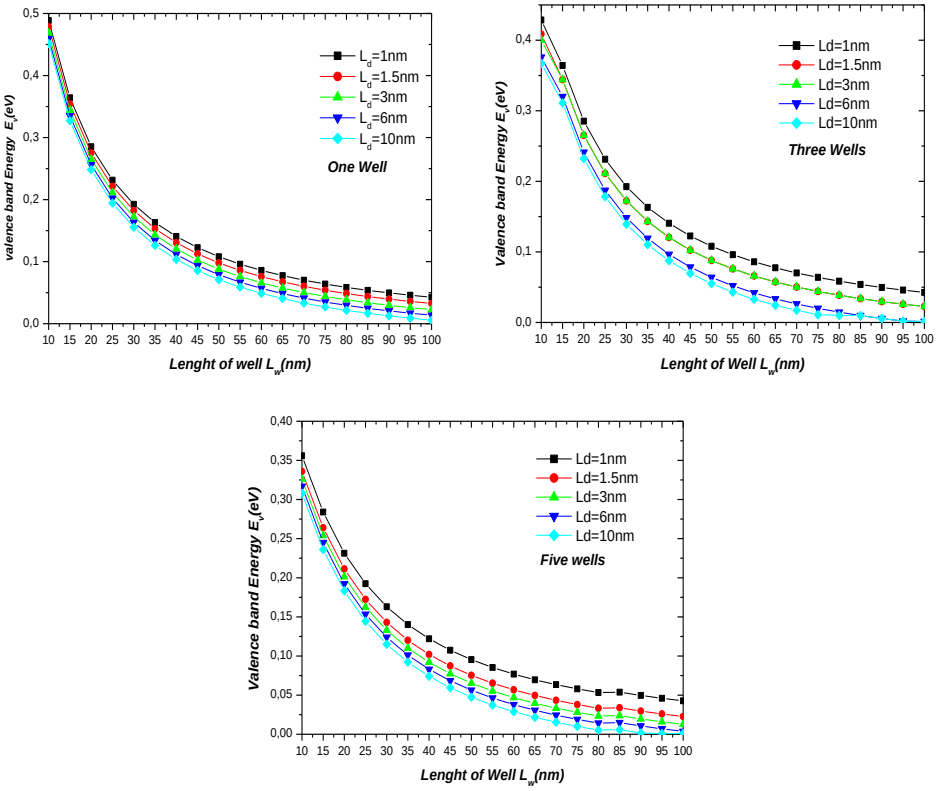

Fig. 4. Valence band Energy of carriers as a function of the barrier width, the well and the number of the wells for $Al_{0.8}In_{0.2}As$ / $Ga_{0.42}In_{0.58}As$ / $Al_{0.8}In_{0.2}As$ structure.

Figs. 5a to 5e determine the value of the effective energy of for bidden band in several wells (M = 1,2,3,4,5) as a function of the thickness of the well and for barriers ranging from 1 to 10 nm . The results obtained show that the Quantum Well based on $Al_{0.8}In_{0.2}As$ / $Ga_{0.42}In_{0.58}As$ / $Al_{0.8}In_{0.2}As$ makes it possible to obtain effective band gap energies ranging from 0.70 to 2.21 eV.

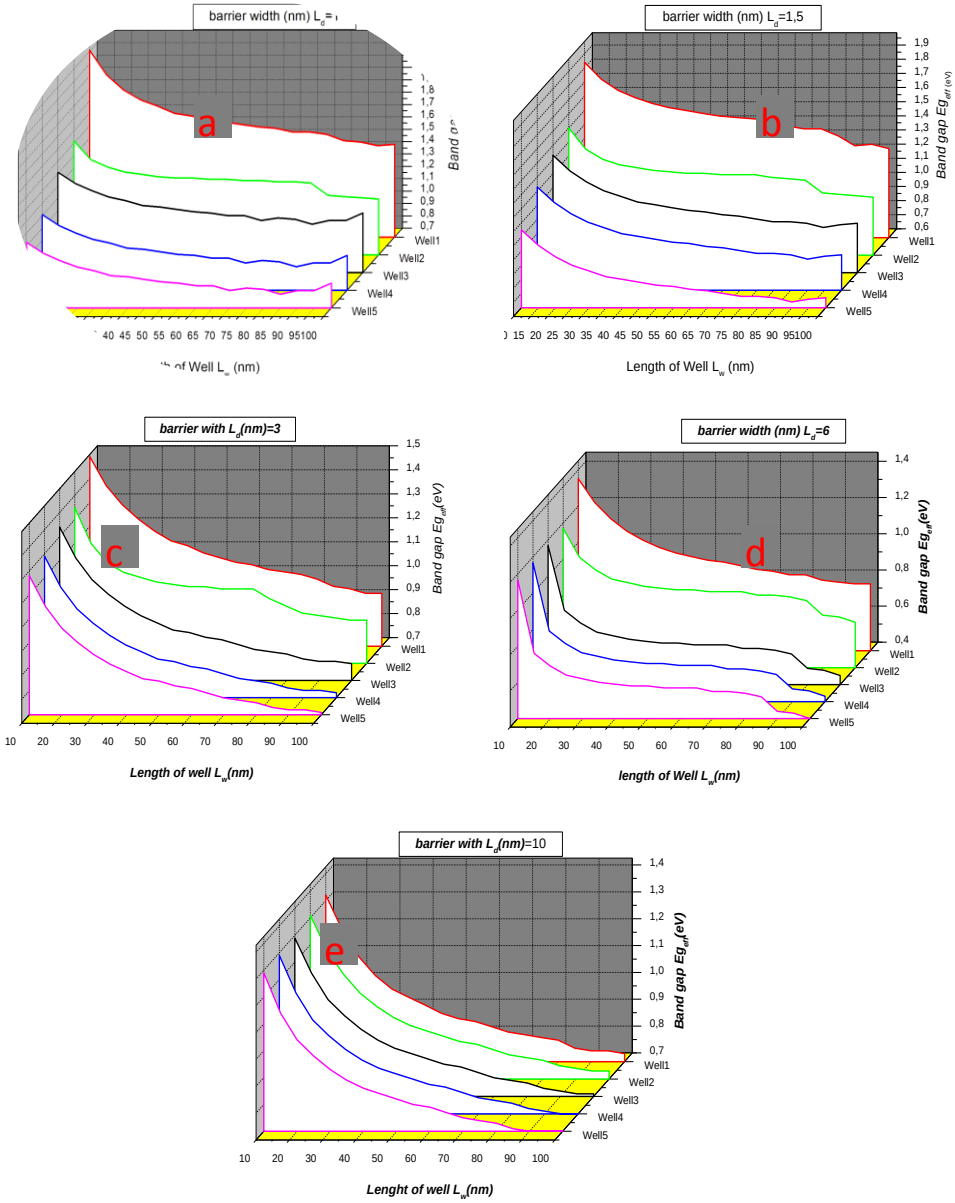

Fig. 5. Effective energy gap of carriers as a function of the barrier width, the well and the number of the wells for $Al_{0.8}In_{0.2}As$ / $Ga_{0.42}In_{0.58}As$ / $Al_{0.8}In_{0.2}As$ structure.

These results show that quantum well parameters and number of wells, they have an impact on the effective energy and solar cell efficiency. The results obtained by the researchers in this field, in particular those obtained by Mr. Green and his team. [9] and those published by Amiri et al [10], support the results presented in the table 2. The values of the forbidden bands are extracted in figure 5, these values allowed us to reach a compilation of up to five junctions with a theoretical yield limit of 57.3%. So, in conclusion, we can theoretically build a tandem solar cell figure 6 achieved the purpose of this work.

Table 2. Band gaps and efficiency for series constrained two-terminal tandem stacks.

Cell	1	2	3	4	5	
	Eg1	*Eg2*	*Eg3*	*Eg4*	*Eg5*	η (%)
	1.34					33 .68
	0.94	1.60				45 .71
	0.93	1.37	1.90			51 .58
	0.71	1.11	1.49	2.00		55.31
	0.70	1.01	1.33	1.67	2.14	57.3

6. Conclusions

Tandem solar cells have the advantage of absorbing the maximum possible of the solar spectrum to have better yields. A quantum well solar cell model was developed and used to theoretically study large qualitative trends in quantum well solar cell performance. The results of this research provide a more complete picture of these devices and should provide a cost-effective guide for its design. The results obtained in this work for an $_8In_{0.2}As$ / $Ga_{0.42}In_{0.58}As$ / $Al_{0.8}In_{0.2}As$ quantum well solar cell at five junctions have the highest efficiency of 57.3%. From these results we can confirm that with a multi-junction cell quantum well will get a better yield, only the manufacture of this kind of structure remains very limited given its complexity.

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