The Study of the Quantitative Properties of the Alloys Ga0.35 in 0.65 As / InP

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Abstract--- The thermal effects on the energy gap and the effect of width of potential well on the quantity properties of hetero-structure nano semiconductors (Ga0.35In0.65As/InP) have been studied.

The energy of quantum wells in conductive and valance bands of alloy has been calculated. Then have been calculated effective energies of transition electronics and associated wavelengths within those well. That was noted the energy gap increases due to reducing temperature to very low degrees also noted the emergence of quantum wells whenever reducing width of potential well to nano dimensions. The results showed that there are improvements in the physical properties of the alloy.

Keywords--- GaInAs, InP, Hetero-structure, Quantum Wells, Energy Gap, Nano Dimensions.

I. INTRODUCTION

A lot of practical and theoretical studies and researches have been done on semiconductor compounds and alloys in recent decades due to their scientific significance and their many applications in various modern devices. Ga0.35In0.65As/InP is a semiconductor material consisting of elements that fall into Group III and V of the periodic table. Semiconductor crystals that have quantum wells are an example of hetero-structure. And it has applications in many fields such as communications, electronics and lasers. Optical Properties of an InGaAs–InP Inter diffused Quantum Well [1].The study of the basic physical properties of In0.53Ga0.47As / InP alloy showed that the energy gap of In0.53Ga0.47As is (eV0.75) and InP is (eV1.34) for a range of wavelengths 1653-925 nm [2]. The crystallization of InGaAs compounds deposited on InP was also studied by STM (Scanning Tunneling Microscopy) technology [3]. As these alloys were used in the design of many devices such as single-photon detection [4], and single-photon avalanche diode [5].

II. THEORETICAL PART

These compositions are prepared with several techniques, the most important of which are (MBE) molecular beam epitaxy and (MOCVD) metal organic chemical vapor deposition. The thickness of the layers prepared with these techniques can be controlled with very high precision (atomic precision). This makes it easy to achieve the thickness of the thin layer needed to obtain the quantum inventory of electrons in the semiconductor at room temperature [6].

Most semiconductor compounds possess a Zinc blend crystal structure, which is face center cubic lattice (fcc). Here, the lattice constants of the constituent components of the alloy must be identical or close together, otherwise

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crystal defects will occur [7]. Where Table-1 gives us the crystal structure and lattice constants of the constituent alloys [8].

Table 1: Crystalline Composition and lattice constants for InP/ Ga_{0.35}In_{0.65}As Alloy Components.

The property	GaAs	InP	InAs	Ga _{0.35} In _{0.65} As
Crystal lattice	Zinc blende	Zinc blende	Zinc blende	Zinc blende
lattice constan	5.65A	5.88A	6.1A	5.88A

The energy gap (Eg) of Ga_{0.35}In_{0.65}As at room temperature can be calculated from the equation:

$$E_a = 0.35 + 0.63x + 0.42x^2 \tag{1}$$

Where x is the ratio of gallium in the compound. For different temperatures, the energy gap is a function of x and T as in equation [9]:

$$E_g(x,T) = 0.42 + 0.625 - \left[\left(\frac{5.8}{T} + 300\right) - \frac{4.19}{T} + 271\right] * 10^{-4}T^2x - (4.19 * \frac{10^{-4}}{T} + 271) + 0.475x^2 \quad (2)$$

The effects of temperature on the energy gap of InP is given using the Varshni equation [10]:

$$E_g(T) = E_g(0) - \frac{\alpha T^2}{T+\beta}$$
(3)

Where Eg (0) is the energy gap at absolute zero, T is the absolute temperature. β and α constants have the values $\alpha = 4.5 * 10^{-4} \text{ eV} / \text{k}$ and $\beta = 327 \text{ K}$ [11].

Figure-1 A square quantum well representing the quantum states (E_e) in the conduction bands and (E_{hh} , E_{lh}) in the valence bands. It also shows the width of the well voltage L_z . (ΔE_C , ΔE_V) it represents the height of the voltage barrier (band offset). From solving the Schrödinger equation inside a specific quantum well we obtain [7]:

$$\mathbf{E} = \frac{2\hbar^2 \mathbf{x}^2}{m^* \mathbf{L_z}^2} \tag{4}$$

Using $x = \frac{KL_Z}{2}$, the values of E_e, E_{hh} and E_{th} can be found. The effective energies needed for the electron to travel from the valence band to the conduction band are calculated by equations [8]:



Figure 1: Quantitative States in a Square Quantitative Well [10]

$$E_{effect} = E_a + E_e + E_{hh} \tag{5}$$

$$E_{effect} = E_g + E_e + E_{lh} \tag{6}$$

The effective mass of alloy compounds depends on the value of x for Ga_xIn_{1-x}As at 300K shown below [11]:

$$m_{\rm e}^* = m_{\Gamma} \cong 0.023 - 0.037x + 0.00x^2 m_0 \tag{7}$$

$$m_{\rm hh}^* \cong (0.41 - 0.1x)m_0 \tag{8}$$

$$m_{\rm lh}^* \cong (0.026 - 0.056x)m_0 \tag{9}$$

III. CALCULATIONS AND RESULTS

The value of the energy gap was determined at different temperatures and the effective mass of the alloy compounds as shown in Table-2. A band offset was calculated in that alloy where $\Delta E_V = 0.467 \text{ eV}$ and $\Delta E_C = 0.263 \text{ eV}$

Table 2: energy gap and effective mass of alloy compounds at different temperatures

Compounds	m^*_{e1}	m^*_{hh1}	$m^*_{ m lh1}$	<i>E</i> _g (eV) 300K	$E_{\rm g}({\rm eV}){\rm oK}$
Ga _{0.35} In _{0.65} As	0.004m _o	0.375 m _o	$0.006 \ m_{o}$	0.62	0.7
InP	0.08 m _o	0.60 m _o	0.082 m _o	1.351	1.421

Figure-2 shows the effect of temperature increases on the energy gap of heterogeneous semiconductors. When the semiconductor temperature increases, it vibrates the atoms of the material around the crystal lattice balance points. Lead to a decrease in the value of the energy gap. In addition, the boundaries of the energy beams are displaced due to the increase in the movement of atoms and thus lead to the expansion of energy levels. Likewise, the electronic reactions within the crystal lattice are highly dependent on temperatures.



Figure 2: Effect of Temperature Increase on the Energy Gap of Heterogeneous Semiconductors

From Table-3 we notice the effect of reducing the quantum well width on the energy of quantum states inside the well.

As the quantum well width decreases, the energy of quantum states increases. This means that the nanoscale dimensions of the materials change the properties of the materials, such as the electronic transfer characteristic and the density of the states, and thus increase the optical conductivity, electrical conductivity, and absorption.

L _Z (nm)	E _{e1} (eV)	E _{hh1} (eV)	E _{lh1} (eV)
5	0.0051	0.0163	0.0112
10	0.0029	0.0050	0.0056
20	0.0016	0.0014	0.0026

Table 3: Quantum States Energies in Electron Volts and different Values LZ in Nanometers

The values of the energetic energies needed to move the electron from the valence band to the conduction band that achieve the transition condition, as well as the accompanying wavelengths when Lz = 5nm and Lz = 10nm, are shown in Table-4 and Table-5, respectively. Figure-3 the change of the affected energies with the main quantum number when Lz = 20 nm.

The main quantity number N	$E_{effect}(E_{hh} \rightarrow E_e) (eV)$	$\lambda = \frac{hc}{\text{Eg}} \ (nm)$	$E_{effect}(E_{lh} \rightarrow E_e) (eV)$	$\lambda = \frac{hc}{\text{Eg}} \ (nm)$
1	0.641	1934	0.636	1949
2	0.705	1758	0.685	1810
3	0.812	1527	0.766	1618
4	0.962	1288	0.880	1409
5	1.155	1073	1.027	1207
6	-	-	1.206	1027

Table 4: Effective Energies and Wavelengths when Lz = 5nm

Table 5: Effective Energies and Wavelengths when Lz = 10 nm

The main quantity number N	$E_{effect}(E_{hh} \rightarrow E_e) \ (eV)$	$\lambda = \frac{hc}{\text{Eg}} \ (nm)$	$E_{effect}(E_{lh} \rightarrow E_e) \ (eV)$	$\lambda = \frac{hc}{\text{Eg}} \ (nm)$
1	0.628	1974	0.6285	1972
2	0.651	1904	0.654	1896
3	0.691	1794	0.696	1781
4	0.746	1662	0.756	1640
5	0.817	1517	0.832	1490
6	0.904	1371	0.926	1339
7	1.007	1231	1.036	1196
8	1.125	1102	1.164	1065
9	1.26	984	1.308	948



Figure 3: The relationship between Effective Energies and the main Quantum Number

IV. CONCLUSION

The alloy on which the calculations are performed is $Ga_{0.35}In_{0.65}As/InP$ where we observe when the temperature increases the lead to a decrease in the value of the energy gap of the alloy. Also, the quantitative effect of the material appears to decrease the width of the potential well to nanoscale dimensions. We notice at the dimension of 10 nm and 20 nm that there is an abundance of electronic transmission states that includes all wavelengths within which this alloy works, which is very useful for studying the physical properties of it, such as absorptivity, electronic conductivity, density of states, probability of occupancy and concentrations of carriers.

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