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$Al_{0.3}Ga_{0.7}As/GaAs$ Single Quantum Well Transition Energy Calculation

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Abstract

The calculation results of e1-hh1 transition energies of $Al_{0.3}Ga_{0.7}As/GaAs$ single quantum well as various temperatures range from 15 K to 120 K have been improved in this work. Good agreement compared with luminescence data has been obtained when some parameters like effective masses of electron and hole, band offsets were changed.

Introduction

Quantum well devices are much interest in the last decade. There are many reports on the calculation of transition energy of quantum well devices[1],[2],[3],[4],[6]. Pecharapa et al studied the photoluminescence of $Al_{0.3}Ga_{0.7}As/GaAs$ single quantum well as various temperatures range from 15 K to 120 K and calculated the transition energies compared with experimental results. Then, after some discussions we found that we can improve the calculation results by using some parameters from the work of A. B. Dzyubenko[2]. A simple program by MathCad 2000 programming give the more satisfied results for us.

Reviews

We use the well known quantum well model like the figure bellow.

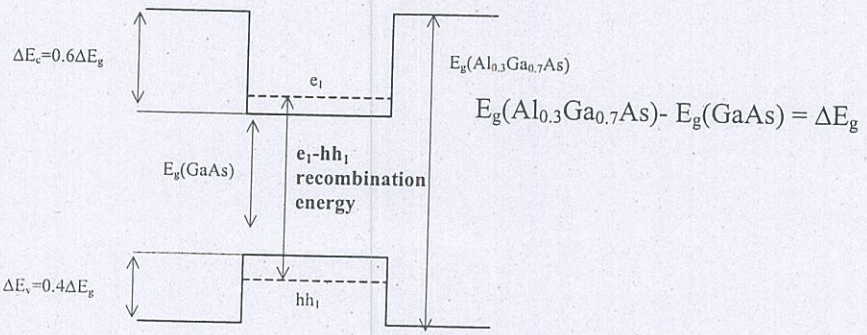

Figure 1 The energy band diagram of $Al_{0.3}Ga_{0.7}As/GaAs$ single quantum well.

$Al_{0.3}Ga_{0.7}As$ barrier GaAs Well $Al_{0.3}Ga_{0.7}As$ barrier

Each energy level e_1 and hh_1 can be calculated from the equation

$$\tan(k_2 a) = \frac{k_1}{k_2} \qquad \text{.....(1)}$$

when a is the half of well width, and

$$k_1 = \frac{2mE}{\hbar^2} \qquad \text{.....(2)}$$

$$k_2 = \frac{2m(v_0 - E)}{\hbar^2} \qquad \text{.....(3)}$$

m is effective mass of the conduction electron or hole, v_0 is the well depth, E is energy level and $\hbar$ = Planck's constant over 2π. Energy level can be obtained by iterating the value of E until the equation (1) is satisfied.

Pecharapa et al [1] used this energy band structure to calculate the transition energy between e_1 and hh_1 and compared results with the experimental data using photoluminescence method. The well width is 20 nm, the well depth is the difference between band gap of GaAs and $Al_{0.3}Ga_{0.7}As$ (figure 1). The energy gap of $Al_xGa_{1-x}As$ at 300K is expressed as,

$$E_g(Al_xGa_{1-x}As) = 1.424 + 1.247(x) \text{ [7]} \qquad \text{.....(4)}$$

While the temperature dependent of energy gap of GaAs is written as

$$E_g(GaAs) = 1.519 - \frac{5.405 \times 10^{-4} T^2}{T + 204} \text{ [5]} \qquad \text{.....(5)}$$

Where T is temperature in Kelvin.

The transition energies were calculated using the energy band model in figure 1 with 20 nm well width. The effective mass of electron (m_e^*) in conduction band is $0.067m_0$ and the effective mass of hole (m_{hh}^*) is $0.45m_0$ [5] when $m_0 = 9.1 \times 10^{-31}$ kg, the band offset $E_c : E_h$ is 60 : 40, are some parameters they used. The compared of the results is shown in the table below.

Table1: Comparison between experimental data using photoluminescence and calculation data.

Temperature (K)	Photoluminescence (eV)	Calculation (eV)	Error (meV)
15	1.526	1.530	4
20	1.524	1.530	6
40	1.523	1.527	4
60	1.521	1.523	2
80	1.517	1.519	2
100	1.513	1.513	0
120	1.510	1.507	3

The New Parameters Calculation

In this calculation, the effective mass of electron(m_e^*) and hole (m_{hh}^*) and the band offset ($E_c : E_h$) were change to $0.067m_0$, $0.35\ m_0$ and 80 : 20 respectively[2]. Then the first energy level in conduction band (e_1) and the first energy level in valence band (hh_1) were calculated as same as the previous calculation. The results from this calculation are closer to the experimental values than the results from Pecharapa et al [1]. The errors shown in table 2 are less than 4 meV.

Table2 The new calculation results.

Temperature (K)	E_{PL} (eV)	$E_{e1\text{-}hh1}$ (eV)	Error (meV)
15	1.526	1.5261	0.08
20	1.524	1.5257	1.71
40	1.523	1.5236	0.58
60	1.521	1.5209	0.08
80	1.517	1.5181	1.08
100	1.513	1.5152	2.23
120	1.509	1.5124	3.44

Discussion

The calculation of the transition energies of quantum well devices $Al_{0.3}Ga_{0.7}As/GaAs$ was performed using MathCad programming. Good agreement with experimental data was shown. More deviated values when temperature increase possibly came from noisy measurements.

Reference

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