Parameter extraction method of band parameters for III-V compound semiconductors using experimental data of transition energies

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Band parameters of group III-V compound semiconductors GaAs, InAs and InP are fitted. Because of the random distribution of elements from the same group within the alloy lattice, exact calculations of material parameters are hardly possible. That is why we tried to fit parameters using as many experimental data as possible. Emphasizing the importance of band structure calculation, direct energy band gap, Passlerr parameters, Luttinger parameters, deformation potentials, energy parameter and correction parameter are fitted, which are the most controversial in literature.

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1. Introduction

At present, III-V compound semiconductor are very important for electronics and optoelectronics devices such as high electron mobility and heterostructure bipolar transistor, laser diodes, light emitting diodes, photodectors, electro-optic modulators and frequency mixing components. As the ternary and quaternary alloys can be found from the binary compounds [1], we need a clear band parameter database.

Band parameters for the III-V semiconductor has been investigated for decades, but these parameters do not have exact theoretical value. Many works have done on these parameters. A comparative survey of experimental and theoretical values of heavy hole and electron effective masses in GaAs, InAs and AlAs was presented by Nakwaski [2]. More than a decade before parameters for all III-V compound semiconductors along with their recommended values and changing area was published [3].

In this present work, we fitted some band parameters of GaAs, InAs and InP for minimizing the difference between theoretical and experimental transition wavelengts. For that we collect some experimental transition wavelengths of InGaAs/GaAs and InGaAs/InP quantum well from different papers.These wavelengths do not match exactly with theoretical model because experimental methods of different references are not same. For that we tried to fit some parameter by finding minimum least square error and calculate the transition wavelegths with these fitting parameters.

2. Theoretical model of transition wavelength calculation

Energy band gap as a function of temperature and carrier concentration can be presented as sum of two components:

$$E_g(T, n_c) = E_g(T) + \Delta E_g(n_c) \tag{1}$$

Band gap reductions with higher temperature mainly arise from the change of the lattice constant. A more accurate physics based formula has recently been proposed by [4].

$$E_g(T) = E(0) - \frac{\alpha\Theta_p}{2}\left[\sqrt[p]{1+\left(\frac{2T}{\Theta_p}\right)^p} - 1\right] \tag{2}$$

$$T = (T_c + T_h)/2 \tag{3}$$

where α is the slope parameter at $T \to \infty$, Θ_p is the average phonon temperature, p is the phonon dispersion parameter.

Quantum levels for the conduction $E_{c,str}$ and valence bands $E_{yy,str}$ can be found as:

$$E^n_{xx,str} = E^n_{xx,b} + \Delta E_{xx,str}. \tag{4}$$

Here *xx = c, hh, lh*.

Including the influence of the barrier [5]:

$$E_{xx,b}^{n} = E_{xx}^{n} n^2 \left(n + \frac{2}{\pi} \sqrt{\frac{m_{xx,b} E_{xx}^{n}}{m_{xx} \left(\Delta E_{xx} + \Delta E_{xx,str} \right)}} \right)^{-2} \quad (5)$$

$$E_{xx}^{n} = \frac{\pi^2 \hbar^2 n^2}{2 m_{xx} t_{qw}^2} \quad (6)$$

where E_{xx}^{n} is the quantum level for an infinite barrier, n is the quantum level number, m_{yy-b} is the effective mass of the barrier.

In most practical cases, conduction band and valence bands can be treated separately. However, one important result relates the electron effective mass to the bulk momentum matrix element which often given in terms of the energy parameter E_p [6]:

$$m_c = \left(\frac{1 + 2F_b}{m_0} + \frac{E_p \left(3E_g + 2\Delta_0 \right)}{3 m_0 E_g \left(E_g + \Delta_0 \right)} \right)^{-1} \quad (7)$$

Here F_b is a correction parameter that accounts for the influence of higher bands, which tend to make the effective mass heavier. ΔE_c and ΔE_v are the potential barrier heights for the conduction and valence bands calculated using the electron affinity as follows [7]:

$$\Delta E_c = \chi_0^{qw} - \chi_0^{bar} \quad (8)$$

$$\Delta E_v = E_g^{bar} - E_g^{qw} - \Delta E_c \quad (9)$$

Alternatively, barrier heights can be found through the model-solid theory, where band structure can be found by the average valence band energy for unstrained semiconductors and split-off energy by [8]:

$$E_{v,av}^{0} = E_v^{0} - \Delta_0 / 3 \quad (10)$$

$$\Delta E_v = E_{v,avg}^{qw} - E_{v,avg}^{bar} + \Delta_0^{qw} / 3 - \Delta_0^{bar} / 3 \quad (11)$$

In case of $\chi_0^A > \chi_0^B$, ΔE_c is positive for type I semiconductor [7]. This structure and the parameters are presented on Fig. 1.

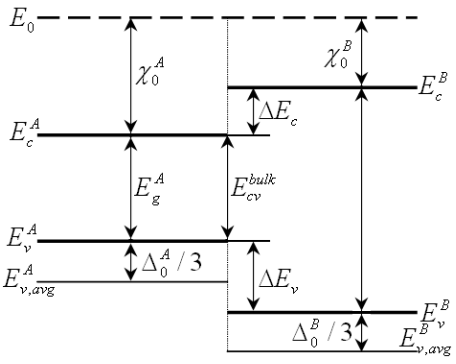

Fig. 1. Band offset parameters for type I junctions. Here A=qw and B=bar.

Strain deforms the crystal lattice. However, it is assumed to be still periodic such that Bloch functions are still applicable. Since the elementary crystal cell is deformed, potential and Bloch lattice functions now have a period equal to the strained elementary cell. The relative change of the lattice period gives the strain [7, 9, 10]:

$$\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{str} = \left(a_0 - a_{qw} \right) / a_w \quad (12)$$

$$a = a + a_T \times 10^{-5} \left(T - 300 \right) \quad (13)$$

The two strain components are related by the elastic stiffness constants C_{11} and C_{12} as:

$$\varepsilon_{zz} = -2C_{12} / C_{11} \varepsilon_{xx} \quad (14)$$

Additions $P_{\varepsilon,x}$ and Q_ε, are required to the diagonal elements of the two-band Hamiltonian matrix [11]

$$P_{\varepsilon,x} = -a_x \left(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} \right) \quad (15)$$

$$Q_\varepsilon = -0.5b \left(\varepsilon_{xx} + \varepsilon_{yy} - 2\varepsilon_{zz} \right) \quad (16)$$

where ε_{xx}, ε_{yy}, ε_{zz} and ε_{str} -strain components in all directions; a_{qw} and a_0-lattice constants of QW and substrate; a_T is the temperature expansion coefficient; a_c and a_v are so-called hydrostatic deformation potentials; b_v is the shear deformation potential.

As a result of this modification, the strain is found to cause the following shifts $\Delta E_{yy,str}$ of the CB and HHB edges at the Γ point.

$$\Delta E_{c,str} = P_{\varepsilon,c} \quad (17)$$

$$\Delta E_{hh,str} = -P_{\varepsilon,v} - Q_\varepsilon \quad (18)$$

The strain including the spin degeneracy [12] results in the following shifts of the light-hole band edges at the Γ point

$$\Delta E_{lh,str} = -P_{\varepsilon,v} + 0.5 \left[Q_\varepsilon - \Delta_0 + \sqrt{\Delta_0^2 + 9Q_\varepsilon^2 + 2Q_\varepsilon \Delta_0} \right] \quad (19)$$

In the k_z direction, bands are still parabolic with effective masses identical to the unstrained case:

$$m_{hh}^z = m_0 \left(\gamma_1 - 2\gamma_2 \right)^{-1} \quad (20)$$

$$m_{lh}^z = m_0 \left(\gamma_1 + 2\gamma_2 f_+ \right)^{-1} \quad (21)$$

Here $f_\pm$ - the strain factor including spin degeneracy

$$f_{\pm} = \frac{2s\left[1+1.5k_{\pm}\right]+6s^2}{0.75k_{\pm}^2 + k_{\pm} - 3s^2} \tag{22}$$

$$k_{\pm} = s - 1 \pm \sqrt{1+2s+9s^2} \tag{23}$$

$$s = Q_{\varepsilon} / \Delta_0 \tag{24}$$

Without strain, s=0 and f=1, the effective masses for heavy and light holes are identical to those obtained from the 4 × 4 Hamiltonian [10].

The final energy levels positions for conduction band are

$$E^n_{c,str} = E^n_{c,b} + E^{qw}_g \quad \text{for type I semiconductor} \tag{25}$$

And for valence band

$$E^n_{hh,str} = E^n_{hh,b} - \Delta E_{hh,str} \tag{26}$$

$$E^n_{lh,str} = E^n_{lh,b} - \Delta E_{lh,str} \tag{27}$$

Assuming the transitions from subbands with the same quantum numbers (k-selection):

$$E^n_{c-yy} = E^n_{c,str} + E^n_{yy,str} \tag{28}$$

Depending of strain type (compressive or tensile) lowest transition will be conduction-heavy hole (c-hh) or conduction-light hole (c-lh), respectively. Finally, expression for transition energy can be described as:

$$E_{tran} = \min\left(E^1_{c-hh}, E^1_{c-lh}\right) \tag{29}$$

And transition wavelength

$$\lambda\left(\mu m\right) = 1.242 / E_{tran}\left(eV\right) \tag{30}$$

Parameters of ternary alloys T_{ABC} $A_xB_{1-x}C$ are usually given as linear interpolation of binary alloys with an empirical bowing parameter C_{ABC} [1]:

$$T_{ABC}\left(x\right) = xB_{AB} + \left(1-x\right)B_{AC} - x\left(1-x\right)C_{ABC} \tag{31}$$

3. Experimental data description

In order to fit band parameters we collect experimental transition wavelength for two different heterostructure configurations, $In_xGa_{1-x}As/GaAs$ and $In_xGa_{1-x}As/InP$. Both heterojunction are fitting simultaneously to get more stable output parameters. Wavelengths are collected with different temperature, material composition and well thickness, because any of these can change the photoluminescence spectra as well as the lasing wavelength of the devices.

For instance changing the In composition from x=0.48 to 0.62 results the change in the lasing wavelength from 1.45 μm to 1.62 μm [23].

We collect total 31 points, 19 ones for the $In_xGa_{1-x}As/GaAs$ quantum well, as shown in Table 1, and 12 ones for $In_xGa_{1-x}As/InP$ quantum well, as shown in Table 2. All parameters in tables are sorted by material composition.

Table 1. Experimental wavelengths from different temperature, In composition and quantum well thickness of InGaAs/GaAs.

Temperature (K)	Material composition	Thickness of The QW(nm)	Wavelength (μm)	References
5	0.10	6.0	0.862	[13]
5	0.15	6.0	0.898	[13]
300	0.17	6.0	0.976	[16]
300	0.20	5.9	1.04	[14]
5	0.20	6.0	0.92	[13]
5	0.25	6.0	0.949	[13]
5	0.30	6.0	1.021	[13]
12	0.30	5.0	0.962	[20]
5	0.35	6.0	1.099	[13]
300	0.35	8.0	1.16	[19]
300	0.36	7.0	1.12	[17]
291	0.388	8.8	1.244	[15]
300	0.40	6.0	1.21	[19]
300	0.42	7.0	1.245	[18]
300	0.45	7.0	1.234	[17]
10	0.475	7.0	1.15	[17]
300	0.48	7.0	1.25	[17]
77	0.50	3.6	1.06	[21]
300	0.50	7.0	1.31	[17]

As ternary $In_xGa_{1-x}As$ are given as linear interpolation of the InAs and GaAs and InP parameters are related for barrier material through eq. (5) and (11), so we can fit band parameters for three binary compound semiconductor GaAs, InAs and InP.

Using the experimental and theoretical wavelengths, we fit the parameters using Levenberg - Marquardt method for the non-linear least-squares [25] which is mathematically defined as

$$R = \sum\left(X_{\exp} - X_{cal}\right)^2 \tag{32}$$

where, $X_{\exp}$ is the experimental wavelength and X_{cal} is the theoretical wavelength.

Then we find the fitted parameter by introducing the fitting coefficients as;

$$P_{aft} = k_{par} \times P_{bef} \tag{33}$$

where, P_{aft} and P_{bef} are the parameters after and before fitting, respectively.

Table 2. Experimental wavelengths from different temperature, In composition and quantum well thickness of InGaAs/InP.

Temperature (K)	Material composition	Thickness of the WQ(nm)	Wavelength (μm)	References
77	0.38	5	1.280	[22]
300	0.46	5	1.428	[23]
300	0.48	5	1.449	[23]
300	0.49	5	1.462	[23]
4	0.53	1.5	1.134	[24]
4	0.53	2.5	1.248	[24]
77	0.53	5	1.393	[22]
4	0.53	8	1.395	[24]
4	0.53	16	1.478	[24]
300	0.55	6	1.568	[23]
300	0.62	5	1.619	[23]
77	0.68	5	1.555	[22]

In Table 3, we putted the parameters for *GaAs*, *InAs* and *InP* before and after fitting with their changing area that we got from [3]. We fitted the direct energy band gap E_g at 0K, Passlerr parameters P, α and Θ which are important for finding energy band gap at 300 K, Luttinger parameters γ_1, γ_2, Deformation potentials $a_{c,}\, a_v$ and b_v important when considering strain effect, interband transition matrix element E_p and the associated F parameter which account for the remote band effects in eight band k.p method.

Table 3. Table for parameters of GaAs, InAs and InP before and after fitting.

Parameter	**GaAs**			**InAs**			**InP**		
	Parameter Before fitting	Changing Area	Fitted Parameter	Parameter Before fitting	Changing Area	Fitted Parameter	Parameter Before fitting	Changing Area	Fitted Parameter
$E_g^{\Gamma}(0K)$	1.519	1.515-1.52	1.52	0.414	0.41-0.45	0.434	1.424	1.420-1.432	1.382
P	2.44	-	3.05	2.1	-	1.68	2.51	-	2.26
α	0.472	-	0.452	0.281	-	0.26	0.391	-	0.488
Θ	230	-	76	143	-	58	243	-	219
γ_1	6.98	6.79-7.20	8.72	20.4	6.79-7.20	18.63	5.06	4.61-6.28	6.06
γ_2	2.06	1.90-2.88	1.65	8.5	1.90-2.88	8.82	1.64	0.94-2.08	2.05
E_p	28.8	25.5-29.0	36	21.5	21.5-22.2	17.23	20.7	16.6-20.7	17.1
F	-1.94	0.76-(-2)	-1.75	-2.9	0-(-2.9)	-4.33	-1.31	0-(-1.31)	-1.56
a_c	-7.17	-6.3-(-18.3)	-6.31	-5.08	-5.08-(-11.7)	-4.11	-6.0	-	-
a_v	-1.16	-0.2-(-2.1)	-0.452	-1	-1.0-(-5.2)	-5.2	-0.6	-	-
b_v	-2.0	-1.66-(-3.9)	-3.63	-1.8	-8-(-2.57)	-1.45	-2.0	-	-

All the parameter fitted here are very important for band structure calculation and often the most controversial. We assume that the barrier has no strain, so we do not fit strain parameters $a_{c,} a_v$ and b_v for InP material.

Results are shown in Fig. 2. The dashed and solid line are presented calculation with parameters before and after fitting respectively, and experimental data are shown by circles.

Fig. 3 shows fitting results for different values of bowing parameter for E_g in InGaAs material.Result show minimum of error at value of 0.477 that is close to result presented in [7].

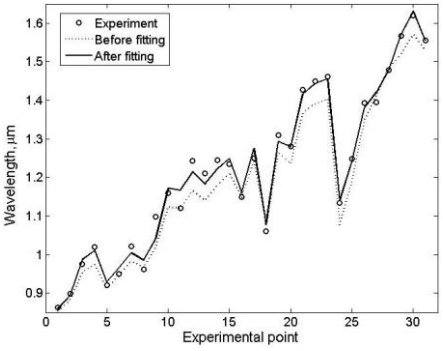

Fig. 2. Fitting results.

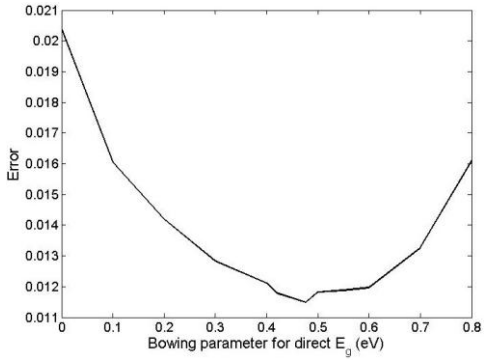

Fig. 3. Error fitting for different bowing parameters of direct band gap.

Other bowing parameters (Fig. 4) do not show any systematic decreasing of error. The fitting of the bowing parameters show an error less than 10^{-4}, so we can assume a linear interpolation for them.

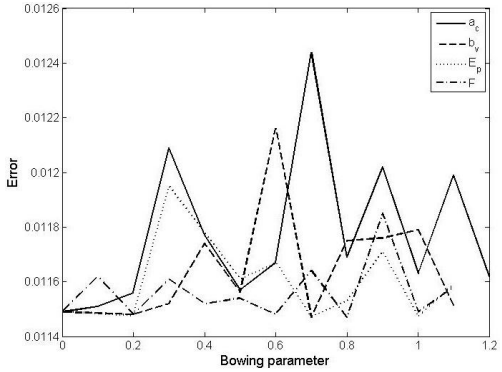

Fig. 4. Fitting errors for bowing parameters.

4. Conclusions

We present an original extraction method that allows receiving more exact set of parameters for three group III-V compound semiconductors GaAs, InAs and InP whose do not have exact theoretical value. Result shows that for most of the experimental transition wavelength, theoretical wavelengths are very close after fitting the band parameter than before fitting. Analysis of bowing parameters for InGaAs material confirms assumption of linear interpolation for all values except of energy band gap.

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