Universal Journal of Electrical and Electronic Engineering 6(5B): 90-95, 2019 http://www.hrpub.org
DOI: 10.13189/ujeee.2019.061612

Band Anti-Crossing Modelling on Tailored $Ga_{1-x}In_xN_yAs_{1-y}$ Band Gap Energy Based Nitrogen Fraction

Muhammad Izzuddin Abd Samad[1,2], Khairul Anuar Mohamad[1,2,*], Mohammad Syahmi Nordin[3], Nafarizal Nayan[1,2], Afishah Alias[2,4], Marinah Othman[5], Adrian Boland-Thoms[3], Anthony John Vickers[3]

[1]Faculty of Electrical and Electronic Engineering, Universiti Tun Hussein Onn Malaysia, Malaysia
[2]Microelectronics and Nanotechnology – Shamsuddin Research Centre, Universiti Tun Hussein Onn Malaysia, Malaysia
[3]School of Computer Science and Electronic Engineering, University of Essex, United Kingdom
[4]Faculty of Applied Science and Technology, Universiti Tun Hussein Onn Malaysia, Malaysia
[5]Faculty of Engineering and Built Environment, Universiti Sains Islam Malaysia, Malaysia

Received August 1, 2019; Revised September 25, 2019; Accepted December 10, 2019

Abstract This paper deals with a Band Anti-Crossing (BAC) modelling to investigate the tailoring of band gap energy of $Ga_{1-x}In_xN_yAs_{1-y}$ alloy based on nitrogen fractions. Three different numerical methods have been adopted to estimate the extended state of conduction band (E_M) parameters. The first two methods used Vegard's law and Varshni's equation to estimate E_M by considering $Ga_{1-x}In_xAs$ as ternary alloy based on temperature dependence, with values of bowing parameter of 0.475 and 0.477, respectively. The third method used excitonic band gap theory for $Ga_{1-x}In_xAs$ alloy temperature dependence by considering Passler fitting (p) and average phonon temperature (θ). Results depict that optimum nitrogen fraction was in the range of 0.012 to 0.018% to achieve the device response at 1.3 μm wavelength, with an energy band gap in range of 0.955 ± 0.005 eV. Future work shows a potential study on influence of indium fractions in tailored energy band gap of $Ga_{1-x}In_xN_yAs_{1-y}$ alloy and compressive strain of material.

Keywords Band Anti-Crossing, Dilute Nitride, Gallium Arsenide, $Ga_{1-x}In_xN_yAs_{1-y}$ Alloy, Band Gap, 1.3 μm Wavelength

1. Introduction

Modern $Ga_{1-x}In_xN_yAs_{1-y}$ semiconductor devices outperform silicon and germanium based on electronics due to their ability to operate at longer wavelengths and direct band gap properties [1]. $Ga_{1-x}In_xN_yAs_{1-y}$ /GaAs offers a much larger conduction band offset due to decreased curvature of the new conduction band in dilute nitrides [2]. Therefore, $Ga_{1-x}In_xN_yAs_{1-y}$ can provide better confinement carriers in quantized sub-bands. They also make a better match of the valence and conduction band densities of states with consequently increased electron effective mass [3]. Utilization of $Ga_{1-x}In_xN_yAs_{1-y}$ based devices in telecommunication application in replacement a current GaInAs/InP-based device, due to their reduced temperature sensitivity and improve refractive index material [1].

An incorporation of a small amount nitrogen into $Ga_{1-x}In_xN_yAs_{1-y}$ based device, offers the flexibility of tailoring energy band gap onto nearest 0.95 eV and lattice-match due to GaAs substrate [4]. Moreover, this addition of nitrogen affected the nonlinear pressure dependence of the band gap [5], a large redshift of the band gap [2], an increase in the electron effective mass [1] and the formation of new bands with strong line width broadened transitions [6]. Many analytical methods are used to understand the effect of nitrogen fraction in $Ga_{1-x}In_xN_yAs_{1-y}$ alloy, such as virtual crystal approximation (VCA) and band anti-crossing (BAC) methods [4].

This study focuses on the dependence of energy band gap and operational wavelength on temperature. The BAC method has been adopted for $Ga_{1-x}In_xN_yAs_{1-y}$ material with constant indium (In) at 0.32% and different nitrogen (N) concentrations ranging from 1.0 to 2.0% with 0.1% increments. BAC simulation method has been developed using MATLAB as a mathematical platform. There are three different numerical techniques to estimate the extended state of conduction band. The first two techniques

use the Vegard's law, while considering the $Ga_{1-x}In_xAs$ material as ternary alloy with different bowing parameters. The third technique uses excitonic band gap theory of $Ga_{1-x}In_xAs$ alloy on temperature dependence. All the numerical methods used the Varshni's equation to determine the equivalent extended states in the conduction band parameter in calculating an eigenvalue of BAC method.

2. Materials and Methods

This is a theoretical approach method that explains the optical bowing in dilute nitride alloys. It describes a variety of experimental phenomena such as band edge energies [7], annealing effect [8], pressure dependence of band gap [5], properties of dilute nitrides and other mismatched alloys. In addition, it could be used to calculate the strength of optical transition in bulk materials and electronic states of quantum wells [3].

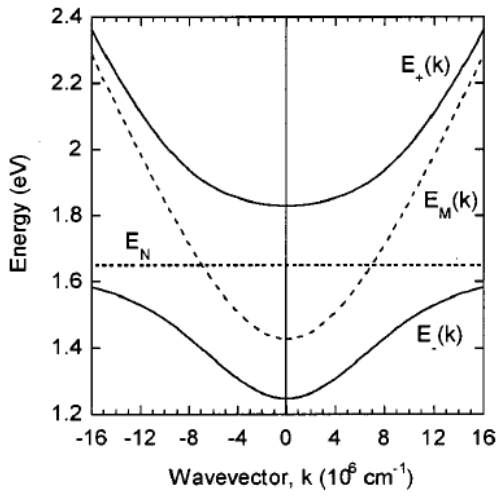


Figure 1. Dispersion relation of the conduction band structure of $Ga_{0.68}In_{0.3}NAs$ near the Γ- point (k = 0) calculated with the BAC method. The dotted lines represent the unpertuned of the N level (En) and the GaAs matrix [2].

The BAC method of $Ga_{1-x}In_xN_yAs_{1-y}$ alloy explained the electronic structure by interaction of elongated conduction-band and localized nitrogen impurity states. This resulted in the splitting of conduction band to blue-shift transition (E_+) and red-shift transition (E_-) bands as shown in Figure 1 [2]. It occurred when the extended states in the conduction band (E_M) and the nitrogen localized state (E_N) are empowered. The approximated solution of this coupling between the two states is established from the two-state-like eigenvalue as,

$$H_{BAC(y)} = \begin{pmatrix} E_M & V_{NM} \\ V_{NM} & E_N \end{pmatrix} \quad (1)$$

Under the assumption of low nitrogen concentration in the group V sub-lattice sites,

$$V_{NM} = C_{NM}\sqrt{y} \quad (2)$$

where C_{NM} is the coupling parameter based on the combination of valance bands and conduction bands of extended heavy hole (HH), light hole (LH) and spin-orbit-split-off (SO) states. The variable y represents nitrogen concentration in the dilute nitride alloy [9]. The parametric values of C_{NM}, E_N and E_M are required for BAC modelling, in order to obtain energy band gap equivalent of $Ga_{1-x}In_xN_yAs_{1-y}$ alloy up to 1.3 μm wavelength. Equation (3) and (4) are widely used in BAC modelling to calculate the value of C_{NM} and E_N for $Ga_{1-x}In_xN_yAs_{1-y}$ alloy [2, 5].

$$C_{NM} = 2.3(1-x) + 1.9x - 4.2x(1-x) \quad (3)$$

$$E_N = 1.7 + 3.89y \quad (4)$$

where x is the In fraction and y is the N fraction. Meanwhile, it is crucial to determine the extended state in the conduction band (E_M) of $Ga_{1-x}In_xAs$, it will be determined through the temperature dependence of $Ga_{1-x}In_xAs$ alloy. There are three different numerical methods that are used to calculate the values of E_M, first two methods use empirical expressions for the ternary alloy composition and temperature dependence based on Vegard's law and Varshni's equations respectively [8]. The third numerical (TM) method utilizes excitonic band gap dependence on temperature for $Ga_{1-x}In_xAs$ alloys [7].

$$E_{a_{1-x}b_xc} = A + Bx - Cx(1-x) \quad (5)$$

where A = E_{bc} and B = $E_{ac} + E_{bc}$ and C is bowing parameter. Equation (5) can be rewritten for $Ga_xIn_{1-x}As$ as a function of gallium fraction (g) with equivalent 1-x and temperature (T) as follows.

$$E_{Ga_{1-x}In_xAs} = E_{InAs}(T) + [E_{GaAs}(T) + E_{InAs}(T)]g - Cg(1-g) \quad (6)$$

Using Varshni's equation to obtain an empirical expression with temperature dependence condition.

$$E_g(T) = E_o(T=0) - \frac{\alpha T^2}{T+\beta} \quad (7)$$

$$E_{Ga_{1-x}In_xAs}(T) = E_{InAs}(0) - \frac{\alpha_{InAs}T^2}{T+\beta_{InAs}} + \left[E_{GaAs}(0) - \frac{\alpha_{InAs}T^2}{T+\beta_{GaAs}} - E_{InAs}(0) + \frac{\alpha_{GaAs}T^2}{T+\beta_{GaAs}}\right]g - Cg(1-g) \quad (8)$$

where α is the limiting slope of band gap shift at high temperature, $E_g(T)$ is the band gap at a finite temperature, E_o is the band gap at 0 ℃ and β is the Deybe temperature of material. The Deybe's temperature values of (8) are listed in Table 1.

Table 1. Material parameters for first and second numerical methods [10].

Material	$E_g(T=0)eV$	α (meV/K)	β (K)
GaAs	1.52	5.8	300
InAs	0.42	4.9	271

$$E_{GaInAs}(g,T) = 0.42 + 0.625.g - \left\{\left[\frac{5.8}{(T+300)} - \frac{4.19}{(T+217)}\right].10^{-4}.T^2.(g)\right\} - \left[\frac{4.19x10^{-4}}{(T+217)}\right].T^2 + Cg^2 \quad (9)$$

$$E_{GaInAs}(1-x,T) = 0.42 + 0.625.(1-x) - \left\{\left[\frac{5.8}{(T+300)} - \frac{4.19}{(T+217)}\right].10^{-4}.T^2.(1-x)\right\} - \left[\frac{4.19x10^{-4}}{(T+217)}\right].T^2 + C.(1-x)^2 \quad (10)$$

For the first method (FM), the value of 0.475 as the bowing parameter is used in the following [9].

$$E_{GaInAs1}(x,T) = 0.42 + 0.625.(1-x) - \left\{\left[\frac{5.8}{(T+300)} - \frac{4.19}{(T+217)}\right].10^{-4}.T^2.(1-x)\right\} - \left[\frac{4.19x10^{-4}}{(T+217)}\right].T^2 + 0.475.(1-x)^2 \quad (11)$$

The second method (SM) used the value of 0.477 as the bowing parameter for following [5].

$$E_{GaInAs2}(x,T) = 0.42 + 0.625.(1-x) - \left\{\left[\frac{5.8}{(T+300)} - \frac{4.19}{(T+217)}\right].10^{-4}.T^2.(1-x)\right\} - \left[\frac{4.19x10^{-4}}{(T+217)}\right].T^2 + 0.477.(1-x)^2 \quad (12)$$

The third numerical (TM) method utilized excitonic band gap in $Ga_{1-x}In_xAs$ alloy with temperature dependence as follows.

$$E_g(T) = E_o(T=0) - \frac{\alpha_p\theta}{2}\left[\sqrt[p]{1+\left(\frac{2T}{\theta}\right)^p} - 1\right] \quad (13)$$

where p is Passler fitting parameter and θ is a constant that is closely related with average phonon temperature. The values of p and θ for (13) are listed in Table 2.

Table 2. Parameters used in the third numerical method [7].

Material	$E_g(T=0)eV$	α_p (meV/K)	θ (K)	p
GaAs	1.52	5.8	230	2.44
InAs	0.42	4.9	143	2.10

The values of C_{NM}, E_N and E_M parameters have been calculated to solve the eigenvalue for (1), in order to predict the splitting of conduction band into two sub-bands, which are the upper E_+ sub-band and lower E_- sub-band as the following [11].

$$E_\pm = \frac{1}{2}\left\{[E_M \pm E_N] \pm \sqrt{[E_M \pm E_N]^2 + 4V_{NM}^2}\right\} \quad (14)$$

3. Result and Discussion

Figure 2 shows the nitrogen localized states (E_N) in the range of 0.01 to 0.02 % based on nitrogen fraction, by incrementing 0.001% through (4). The extended states of the conduction band have been obtained by using (12), (13) and (14) as shown in Figure 3.

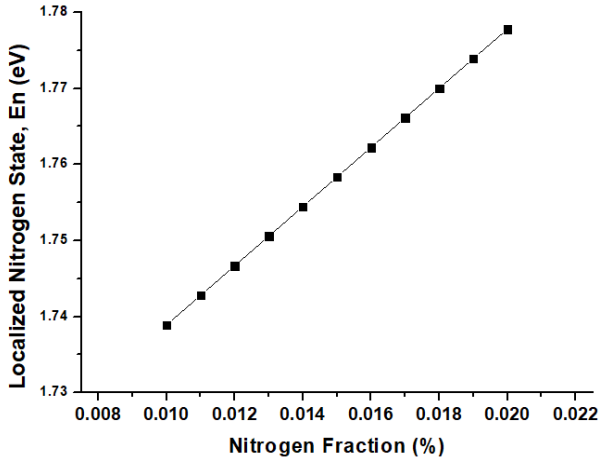


Figure 2. The localized nitrogen energy states in range of 0.01 to 0.02 % by increment of 0.001%, based on nitrogen fraction

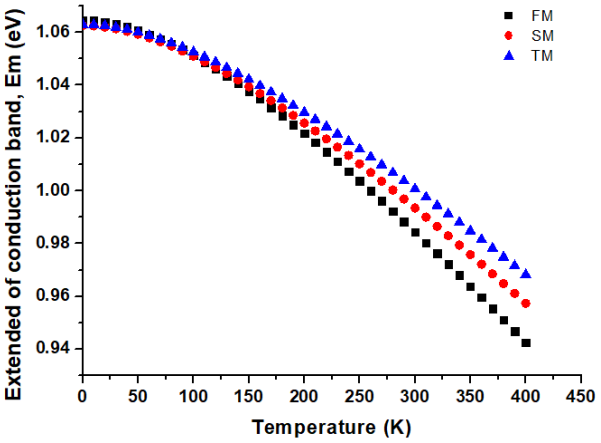
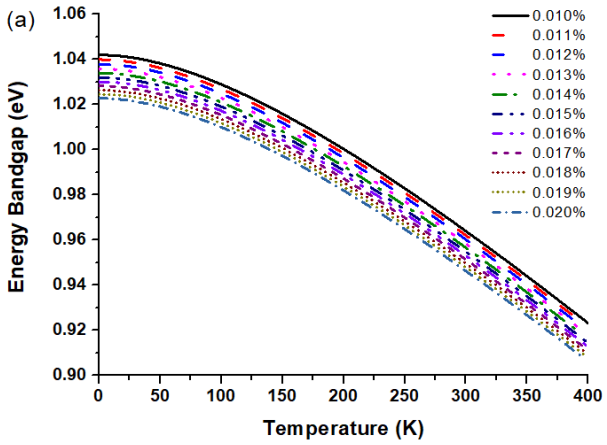
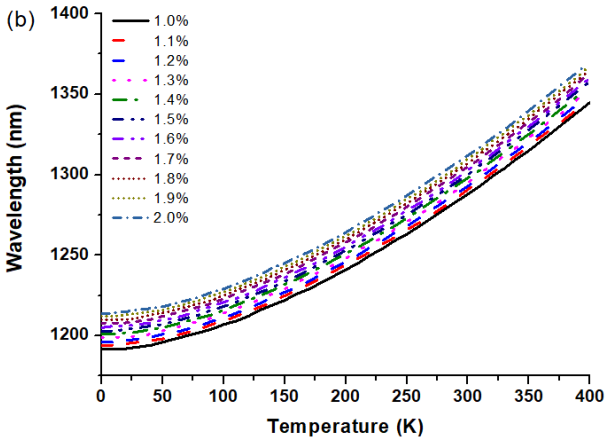


Figure 3. The extension of conduction band by using FM, SM and TM based on temperature dependence from 100 K to 400 K.

The E_N and E_M parameters have been used to calculate the eigenvalues of (1). Equation (14) is solved to obtain the band gap energy of $Ga_{1-x}In_xAs$ alloy and wavelength as shown in Figure 4, Figure 5 and Figure 6.





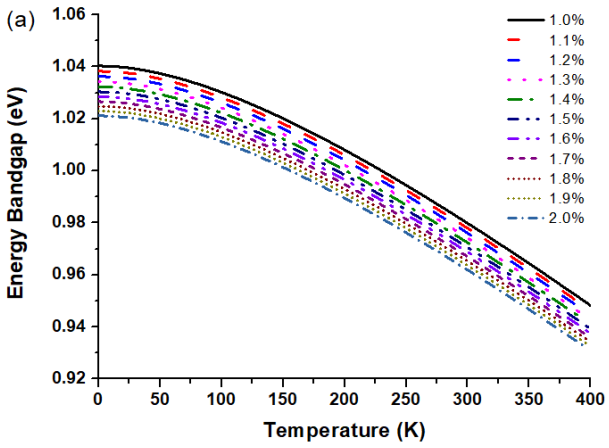
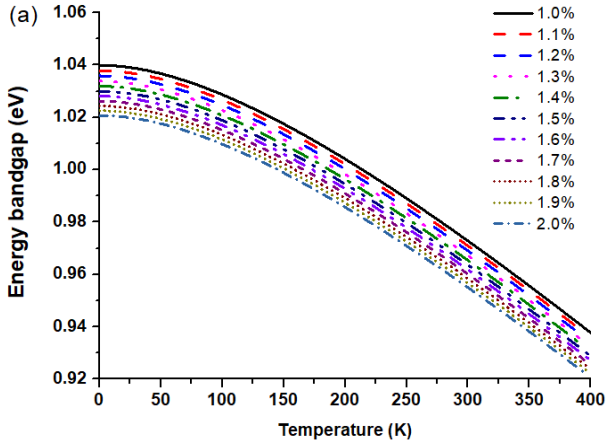


Figure 4. Temperature dependence of $Ga_{1-x}In_xN_yAs_{1-y}$ alloy (a) energy band gap (b) wavelength by using FM BAC method.



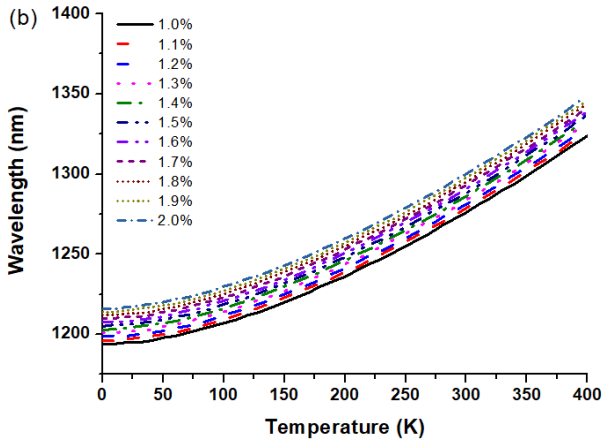


Figure 5. Temperature dependence of $Ga_{1-x}In_xN_yAs_{1-y}$ alloy (a) energy band gap (b) wavelength by using SM BAC method.

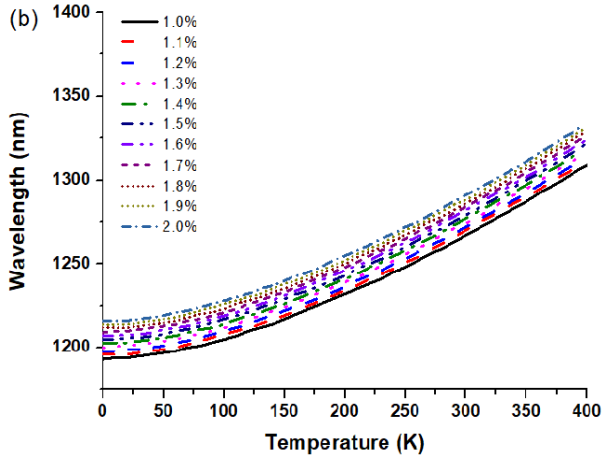
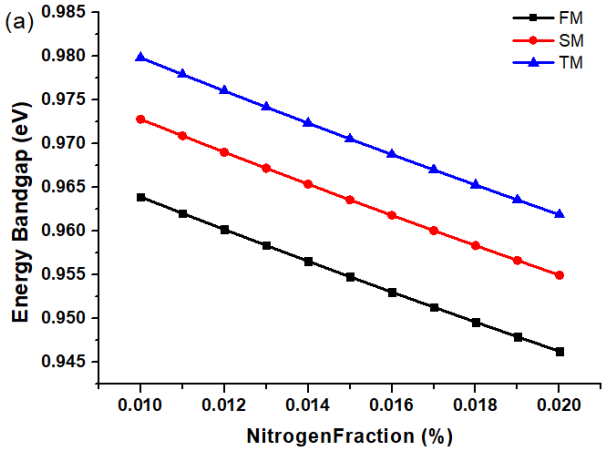


Figure 6. Temperature dependence of $Ga_{1-x}In_xN_yAs_{1-y}$ alloy (a) energy band gap (b) wavelength by using TM BAC method.



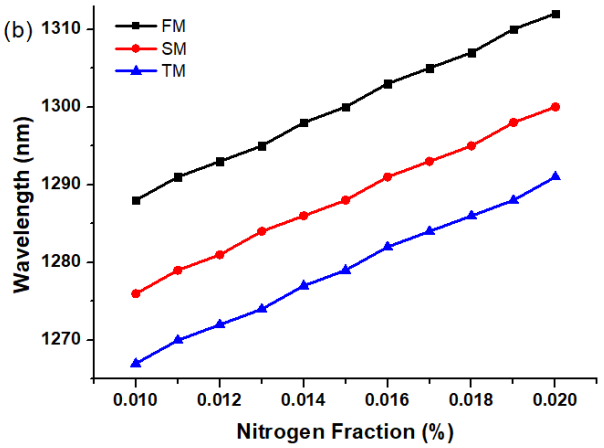


Figure 7. BAC results (a) energy band gap (b) wavelength of $Ga_{1-x}In_xN_yAs_{1-y}$ alloy at 300K.

The energy band gap and wavelength at 300 K are shown in Figure 7 which visualizes the increment energy band gap and wavelength based on the nitrogen fraction for each method.

Table 3. The energy band gap of $Ga_{1-x}In_xN_yAs_{1-y}$ alloy at 300 K for each method

Nitrogen Fraction (%)	Energy Band Gap (eV)		
	FM	SM	TM
1.0	0.964	0.973	0.980
1.1	0.962	0.971	0.978
1.2	0.960	0.969	0.976
1.3	0.958	0.967	0.974
1.4	0.957	0.965	0.972
1.5	0.955	0.964	0.971
1.6	0.953	0.962	0.969
1.7	0.951	0.960	0.967
1.8	0.950	0.958	0.965
1.9	0.948	0.957	0.964
2.0	0.946	0.955	0.962

As shown in Table 3, the energy band gap of $Ga_{1-x}In_xN_yAs_{1-y}$ alloy at 300 K offers a lower deviation at 0.964 ± 0.01 eV based on the nitrogen fraction. The deviation of energy band gap for FM and SM is influenced by the bowing parameters of Vegard's law used to accommodate the curvature of extended conduction band energy. The deviation of wavelength in Table 4 also depicts a similar trend with the energy band gap.

Table 4. The wavelength of $Ga_{1-x}In_xN_yAs_{1-y}$ alloy at 300 K for each method

Nitrogen Fraction (%)	Wavelength (nm)		
	FM	SM	TM
1.0	1288	1276	1267
1.1	1291	1279	1270
1.2	1293	1281	1272
1.3	1295	1284	1274
1.4	1298	1286	1277
1.5	1300	1288	1279
1.6	1303	1291	1282
1.7	1305	1293	1284
1.8	1307	1295	1286
1.9	1310	1298	1288
2.0	1312	1300	1291

Based on the FM BAC modelling, it shows the optimum N fraction in range of 0.012% to 0.018% to achieve a response device at 1.3 µm wavelength with energy band gap 0.955 ± 0.005 eV with 1.3 ± 0.005 eV. Meanwhile, the SM and TM results were the outline data on the basic strategies to achieve 1.3 µm emission from $Ga_{1-x}In_xN_yAs_{1-y}$ material with 1.5 ± 0.2 N% fraction [4]. Based on that fraction, the composition of $Ga_{1-x}In_xN_yAs_{1-y}$ material with 32% In with 1.2%-1.8% N was promised the optimum lattice constant and compression strain [1]. In this case, the compression strain of material is dependent on the indium fraction and tensile strain of material is coming from the nitrogen fraction [4].

In other word, the increment of N fraction in host semiconductor material able decreases the material optical quality [3]. In fact, the increment of N fraction restructures the conduction band of the host semiconductor by rising the electron states density at edge conduction band [7]. Restructuring of the conduction band occurs by the delocalized conduction band and localized nitrogen level interaction in host semiconductor material. In addition, the N fraction influences the hole effective mass of material by strain-induced valance band non-parabolicity and it might affect the electrical and optical properties of material [4]. Therefore, there is a potential to study the influence of indium fraction in tailored energy band gap of $Ga_{1-x}In_xN_yAs$ alloy and compressive strain of material.

4. Conclusions

The effect of nitrogen fraction on tailored energy band gap of $Ga_{1-x}In_xN_yAs_{1-y}$ alloy has been investigated by using band anti-crossing (BAC) method based on temperature dependence. This work adopted three numerical methods to determine E_M parameter based on Vegard's law, excitonic band gap and Varshni's equation. Based on BAC results, the optimum nitrogen fraction has been evaluated in the range of 0.012 to 0.018% to achieve a device response at 1.3 μm wavelength with an energy band gap of 0.955 ± 0.005 eV. Thus, it has a potential to study the influence of indium fraction in tailoring energy band gap of $Ga_{1-x}In_xN_yAs_{1-y}$ alloy and compressive strain of material.

Acknowledgements

This work is funded by Research Management Centre, Universiti Tun Hussein Onn Malaysia under TIER 1 (H191) and Postgraduate Research Grant (GPPS-H306). The authors were also thankful to Optoelectronic and Terahertz Research Laboratory at the University of Essex for providing the dilute nitride and gallium arsenide samples.

REFERENCES

[1] F. Sarcan, O. Donmez, M. Gunes, M.C.Arikan, J.Puustinen and M.Gunia, Influence of nitrogen on hole effective mass and hole mobility in p-type modulation doped GaInNAs / GaAs quantum well structures, Applied Physics Letters, Vol. 103, No.8, 082121-082125, 2013

[2] C. Skierbiszewski,a) P. Perlin, P. Wisniewski, W. Knap, T. Susk, W. Walukiewicz, W. Shan, K. M. Yu, J. W. Ager, E. E. Halle, J. F. Geisz and J. M. Olson, Large, nitrogen-induced increase of the electron effective mass in InyGa1−yNxAs1−x, Applied Physics Letters, Vol.76, No.17, 2409–2411, 2000.

[3] S. Shirakata, M. Kondow, and T. Kitatani, Photoluminescence and photoreflectance of GaInNAs single quantum wells, Applied Physics Letters, Vol. 79, No 1 pp. 54–55, 2001.

[4] F. Sarcan, O. Donmez, M. Gunes, A. Erol, M. C. Arikan, and J. Puustinen, An analysis of Hall mobility in as-grown and annealed n- and p-type modulation-doped GaInNAs / GaAs quantum wells, Nanoscale Research Letters, Vol. 7, No. 1 pp. 2–7, 2012.

[5] P. J. Klar and H. Gru, Pressure and temperature dependent studies of GaN x As 1 — x / GaAs quantum well structures, Physics of the Solid State, Vol. 223, No. 1 pp. 163–170, 2001.

[6] C. Skierbiszewski, Experimental studies of the conduction-band structure of GaInNAs alloys, Semiductor Science and Technology., Vol.17, No.8, 2002.

[7] M. Bayer, S. Fafard, and Z. R. Wasilewski, Temperature dependence of the excitonic band gap in In (x) Ga (1-x) As / GaAs self- assembled quantum dots, Physics Review B, Vol.72, No.8, pp. 085328, 2005.

[8] I. Vurgaftman and J. R. Meyer, Band parameters for III – V compound semiconductors and their alloys, Journal of Applied Physics, Vol. 89, No. 11, 2013.

[9] S, Paul., J. B. Roy, and P. K. Basu, Empirical expressions for the alloy composition and temperature dependence of the band gap and intrinsic carrier density in GaxIn1−xAs, Applied Physics Letters, Vol. 69, No. 2 pp. 827-829, 2013.

[10] I. Vurgaftman, J. R. Meyer, I. Vurgaftman, and J. R. Meyer, Band parameters for nitrogen-containing semiconductors, Applied Physics Letters, Vol. 94, N0.6 , 2012.

[11] W. Shan., W. Walukiewicz., K. M. Yu., J. W, Ager Iii., E. E. Haller., J. F. Geisz., D. J. Friedman., J. M. Olson., S.R, Kurtz., H. p. Xin, and C. W. Tu, Band anticrossing in III–N–V alloys. physica status solidi (b), Vol.223, No.1, pp.75-85, 2001.