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A theoretical evaluation of Gallium concentration profile and in-plane strain as a function of growth axis z for different diffusion length L_d and study of energy shift (meV) as a function of annealing temperature of GaInNAs/GaAs quantum well laser

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Abstract: Using the theoretical formalism of ***H D Sun etal [J. of Appl. Phys. 94, 7581 (2003)], A. Mika etal. [Optica Applicata Vol XLIII, No1 (2013)], Y. N. Qiu etal. [Semicond. Sci. Technol. 23, 095010 (2008)] and S. B. Healy etal. [IEE Proc. Optoelectron, 151, 115505(2004)],*** we have theoretically evaluated Ga-concentration profile, in-plane compressive strain of GaInNAs/GaAs quantum well as a function of growth direction z for different diffusion length. Our theoretically obtained results show that concentration profile increase and decrease with z for each value of diffusion length whereas in-plane compressive strain changes from zero to negative value with z for each of the diffusion length taken. These results indicate that with the increase of diffusion length the Gallium element in the barrier penetrates further into the quantum well which makes the gradual change of the element concentration between the barrier and the well. Our in-plane strain calculations show that quaternary alloy GaInNAs is less strained than the ternary alloy GaInAs. This is because the lattice constants of GaN and InN are small. The evaluation also gives an indication that due to compressive strain the hydrostatic component widen the band

gap and the shear strain component enlarge the splitting between the heavy hole (HH) and the light hole (LH) at band edge k=0. Our theoretically obtained results of intensity of normalized PL-spectra as a function of photon energy for two growth samples, as-grown and PECVD grown show that the PL intensity increase and decrease as photon energy. Our obtained results are in good agreement with compositional analysis of SIMS. We have also analysed the experimental data obtained by group led by H. D. Sun etal regarding the energy shift of GaInNAs/GaAs structure as a function of annealing temperature and also for different N-concentrations. Our analysed results show that PL intensity increase with decrease of N-concentrations. These findings not only rules out the possible mechanism of N-As inter-diffusion but also demonstrates the alloy stability of GaInNAs due to strong bond of In-N. Our all analysed experimental results are in good agreement with the other theoretical workers.The entire evaluation is based on Fick's law and BAC model with the help of Luttinger-Kohn Hamiltonian. The validity of the model has been confirmed by the excellent agreement with PLE data. The obtained results will be quite useful in the design of integrated photonic devices based on GaInNAs/GaAs material.

Keywords: Epitaxial crystal growth, Reflectance spectra, Luttinger-Kohn Hamiltonian, BAC (Band-anti-crossing model, Interband relaxation model. Ga-concentration profile, in-plane strain, Intensity of normalized PL-spectra, Plasma enhanced chemical vapour deposition (PECVD) technique, Fick's law, Annealing temperature, PL energy shift, Secondary Ion Mass Spectroscopy (SIMS), Photoluminescence excitation (PLE), Diffusion length, Quaternary alloy, Ternary alloy.

INTRODUCTION

In an earlier paper[1], we have theoretically studied the effect of quantum well intermixing on the material gain of GaInNAs/GaAs quantum well. We have taken theoretical[2-4] formalism to study this effect. We have studied reflectance spectra of this intermixed well as a function of photon energy and also intensity of derivative of the spectra as a function of photon energy in order to know the transmission intensity in such differential spectrum. We have also evaluated optical transition oscillator strength in (a.u.) and square of the overlap integral as a function of photon energy. Our theoretically obtained results show that both increase with photon energy. Our evaluated results of transition energies for different optical transition E1-HH1 (electron and heavy Hole transition) and E1-LH1(electron and light Hole transition) increase with diffusion length (nm). The obtained results are in good agreement with experimental data[5]. We have also evaluated dipole moments of TE and TM polarization for E1-HH1 and E1-LH1 optical transition as a function of wave vector (A^{0-1}) for different diffusion lengths. Our theoretically evaluated results show that for lower values of diffusion length, TE mode decrease and TM mode increase with wave vector (A^{0-1}). However for large diffusion lengths like L_d =4nm, 6nm and 8nm only TE modes decrease but TM modes for both E1-HH1 and E1-LH1 are suppressed. Our theoretically obtained results for TE gain as a function of photon energy and peak of TE gain (cm^{-1}) as a function of carrier density ((cm^{-3}) increase with photon

energy and carrier densities. Our theoretically evaluated results are in good agreement with the other theoretical workers[6-9].

In this paper, we have evaluated concentration profile of GaInNAs along the growth direction z with different diffusion length L_d. Now due to analysis of secondary ion mass spectroscopy (SIMS)[10,11] the diffusion of group III atoms (In and Ga) is assumed and atomic profile after diffusion is modelled using Fick's law[12]. Combined with BAC model[13], one calculates the electronic properties of intermixed GaInNAs/GaAs quantum well. This model is confirmed by the comparision made between calculated transition energies and the optical transition observed by photoluminescence excitation (PLE)[14]. The predicted diffusion length is consistent with the observation of SIMS which further supports the analysis. Our theoretically obtained results of Ga concentration profile of GaInNAs along the growth direction z for different diffusion length L_d show that Ga concentration profile decrease and then increase as a function of diffusion length L_d. The same trend is observed for all the values of L_d taken. Our other evaluation of in-plane strain of GaInNAs/GaAs quantum well structure as a function of growth axis considering N concentration for different values of diffusion length L_d indicate that in-plane compressive strain (%) as a function of z cross from positive to negative values for the values of z from -2 to +2. The same trend is observed for all the values of L_d taken. Our evaluated results of intensity of normalized PL spectra of $Ga_{0.728}In_{0.272}N_{0.0114}As_{0.9886}$/GaAs structure as a function of photon energy (meV) for as-grown sample show that normalized PL intensity (arb. u) increase as a function of photon energy attain a peak and then decrease. We have studied experimental results of energy shift (meV) as a function of annealing temperature (^{0}C).

The results show that the energy shift (meV) increases as a function of annealing temperature from 500^{0}C to 900^{0}C. The experiment was performed by H.D. Sun etal.[15]. The sample was prepared by PECVD-$Si0_2$ method. PECVD stand for Plasma enhanced chemical vapour deposition technique. The other experimental studies were performed for normalized PL-spectra of $Ga_{0.728}In_{0.272}N_{0.0114}As_{0.9886}$/GaAs structure as a function of wavelength (nm) at different annealed temperature for PECVD grown sample. The annealed temperature duration was 180s and the experiment was performed by group led by H.D. Sun etal.[15]. The experimental results were taken for three different annealed temperatures 800^{0}C, 700^{0}C and 650^{0}C. The obtained result shows that PL intensity (arb. U) Increases, attains a peak value and then decreases for the values of the wavelength from 1000nm to 1100nm. Finally, we have studied the experimental results of dependence of PL energy shift of GaInNAs/GaAs structure with different N concentration (%) as a function of annealing temperature for PECVD growth sample. The results were taken for three different N-concentration as N=0.5%, N=0.88% and N=1.14%. The obtained results show that the energy shift (meV) increase for all the values of N-concentration as a function of annealing temperatures starting from 450^{0}C to 1050^{0}C. the obtained results are in good agreement with the other theoretical workers[16-19.]

MATHEMATICAL FORMULAE USED IN THE EVALUATION

Evaluation of Gallium concentration profile in the growth direction for different diffusion length L_d: The Gallium concentration profile along growth direction is evaluated using Fick's law which deals with atomic diffusion. As we all know that quantum well intermixing (QWI) is a process in which atoms move across the hetrostructures from region of high concentration to region of low concentration. The consequent compositional redistribution will change the electronic property of

quantum well material. Based on the observed result of SIMS[10], one assumes that in an intermixed quantum well of GaInNAs the atomic diffusion mainly attributes to group III atoms, Indium and Gallium. Their concentration profile will br described by Fick's second law[12].

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial z^2} \quad \ldots (1)$$

For a constant diffusivity, D, the rate of concentration (C) change is proportional to the concentration gradient $\frac{\partial C}{\partial z}$. One assumes that all the atomic movement is independent of atomic concentration and the diffusion coefficient D is constant. The compositional profile after diffusion is characterized by diffusion length $L_d = (D.t)^{\frac{1}{2}}$. With the as-grown indium mole fraction given by x_0, the indium concentration profile after diffusion can be described by the error function

$$x(z) = \frac{x_0}{2}[erf(\frac{L_z + 2z}{4L_d}) + erf(\frac{L_z - 2z}{4L_d})] \quad \ldots (2)$$

Here L_z is as-grown well width, z is the crystal direction and the quantum well centre is at z=0. The gallium concentration is (1-x(z)) which is the function of the crystal growth direction. Its profile with different diffusion length L_d has been calculated and is shown in table T1. With the increase of the diffusion length L_d, the gallium element in the barrier penetrates into quantum well. This makes the gradual change of element concentration between the barrier and the quantum well. The energy band gap of ternary alloy $In_{x(z)}Ga_{(1-x(z))}As$ has been calculated by the following equation and is in quadratic form[20,21]

$$E_g(\ln GaAs, z) = x(z)\,\mathrm{E}_g(\ln As) + (1 - x(z))E_g(GaAs) - Cx(1 - x(z)) \quad \ldots (3)$$

Here, C is the bowing parameter which accounts for the deviation from a linear interpolation between two binary alloys. Due to compositional diffusion, the energy gap is altered by the compositional profile. Equation (3) gives that the energy band gap is a function of quantum-well growth direction and it is no longer abrupt on the interface. The temperature dependence of the band gaps of binary materials is given by empirical Vashni equation[22,23]

$$E_g(GaAs, T), \mathrm{E}_g(\ln As, T) = E_g(T_0) - \frac{\alpha T^2}{T + \beta_1} \quad \ldots (4)$$

Here, α and β_1 are adjustable Vashni parameters.

Evaluation of strain profile between quantum well and barrier: For the evaluation of strain profile between quantum well and barrier, one takes help of two-band BAC model[24] and a 6x6 Luttinger-Kohn Hamiltonian[25]. The two-band BAC model is applied to calculate band structure of the GaInNAs/GaAs quantum well material. The BAC model treats the interaction of the InGaAs host with the localized N state. It explains the band-gap shrinkage and the non-parabolic conduction band of

dilute nitride[23-25]. In this study, one will investigate whether the BAC model is appropriate to consider intermixing effects. Due to high strain with 38% indium in the quantum well 6x6 Luttinger-Kohn Hamiltonian is used to calculate the valence band. In the BAC model the coupling between the localized state and the GaInAs extended state can be solved by extracting the eigenvalue of the two-band Hamiltonian[23,25]

$$\begin{pmatrix} E_M(y,z)+\frac{h^2k^2}{2m_e} & V_{MN}(y,z) \\ V_{MN}(y,z) & E_N(y,z) \end{pmatrix} \quad \ldots (5)$$

Where $E_M(y,z) = E_{CInGaAs}(z) - 1.55y \qquad z \le |a|$

$= E_{CBarrier}(z) \qquad z > a \quad \ldots (6)$

$E_N(y,z) = 1.52eV - 3.9y \qquad z \le |a|$

$= 1.52eV + 0.22$ z>a … (7)

$V_{MN} = \beta\sqrt{y} \quad \ldots (8)$

$\beta = 1.6 : \ 3.0, \qquad z \le |a|$

=0 z>a … (9)

Here, y is the concentration of nitrogen and z is the growth direction along the quantum well. Due to the high strain in the GaInNAs/GaAs quantum well, it is necessary to include a spin-orbit band into the calculation of the valence band structure. The diagonal form of 6x6 Luttinger-Kohn Hamiltonian[25]

$$H_{3x3} = -\begin{pmatrix} P+Q & -R_\rho - iS_\rho & -\sqrt{2}R_\rho + i/\sqrt{2}S_\rho \\ -R_\rho + iS_\rho & P-Q & \sqrt{2}Q + i\sqrt{3}/\sqrt{2}S_\rho \\ -\sqrt{2}R_\rho - i/\sqrt{2}S_\rho & \sqrt{2}Q - i\sqrt{3}/\sqrt{2}S_\rho & P+\Delta \end{pmatrix} \quad \ldots (10)$$

Here $P = P_k + P_\varepsilon \qquad Q = Q_k + Q_\varepsilon \quad \ldots (11)$

$R = R_k + R_\varepsilon \qquad S = S_k + S_\varepsilon \quad \ldots (12)$

$P_k = (\frac{h^2}{2m_\sigma})\gamma_1(z)(k^2{}_P + k^2{}_z) \qquad P_\varepsilon = H_v(z) \quad \ldots (13)$

$Q_k = (\frac{h^2}{2m_\sigma})\gamma_2(z)(k^2{}_P - 2k^2{}_z) \qquad Q_\varepsilon = S_v(z) \quad \ldots (14)$

$R_\rho = -(\frac{h^2}{2m_\sigma})\sqrt{3}\gamma(z)\,k^2{}_P \quad \ldots (15)$

$$S_{\rho} = (\frac{h^2}{2m_{\sigma}})2\sqrt{3}\gamma_3(z)k_P k_z \quad \ldots (16)$$

Materials parameters such as the effective mass, the Luttinger parameters, the conduction band hydrostatic deformation potential a_c, the valence band hydrostatic deformation potential a_v, the shear deformation potential b and the elastic stiffness constants C_{11} and C_{12} are calculated by interpolation of the binary parameters of InAs and GaAs by the following equation

$$T(In_{x(z)}Ga_{1-x(z)}As) = (1-x(z)B(GaAs) + x(z)B(InAs) \quad \ldots (17)$$

Here, T represents the ternary alloy parameter and B represents the binary parameter. All these parameters are compositional dependence and continuous across the well and barrier. In order to consider the N influence on strain, the lattice constant is calculated in quaternary form:

$$Q(In_{x(z)}Ga_{1-x(z)}N_yAs_{1-y}) = (1-x(z)(1-y)B(GaAs) + x(z)(1-y)B(InAs)$$
$$+(1-x(z))yB(GaN) + x(z)yB(InN) \quad \ldots (18)$$

Here, Q represents the quaternary alloy parameter and y is the concentration of N. It consists of the lattice constant of GaAs(5.65A^0), InAs(6.05A^0), GaN(4.5A^0) and InN(4.98A^0)

It is assumed that the strained layer semiconductor is pseudomorphically grown on a (0 0 1)-oriented substrate so that only the biaxial strain exists

$$\varepsilon_{xx}(z) = \varepsilon_{yy}(z) = \frac{a_s - a_{\omega}(z)}{a_{\omega}(z)} \neq \varepsilon_{zz} \quad \ldots (19)$$

$$\varepsilon_{xy} = \varepsilon_{yz} = \varepsilon_{xz} = 0 \quad \ldots (20)$$

Here, a_s and a_{ω} are the lattice constants of the substrate and well respectively. The strain profile between the quantum well and barrier has been calculated and is shown in table T2. It is shown that the quaternary GaInNAs is less strained than the ternary GaInAs due to the smaller lattice constants of GaN and InN. The softer evolution of the strain within the well and through the strain step at the interface is then observed. Due to the compressive strain, the hydrostatic component will widen the band gap and the shear component will enlarge the splitting between heavy hole (HH) and light hole (LH) at the band edge k=0

$$H_{c,v}(z) = -2a_{c,v}(z)[1-C_{12}(z)/C_{11}(z)]\varepsilon_{xx}(z) \quad \ldots (21)$$

$$S_v(z) = -b(z)[1+C_{12}(z)/C_{11}(z)]\varepsilon_{xx}(z) \quad \ldots (22)$$

Here, indices c and v represent the hydrostatic component of the conduction band and valence band respectively. As the growth direction (z) dependence of all the parameters joins into the calculation of $H_{c,v}$ and S_v which are also functions of z.

DISCUSSION OF RESULTS

sing the theoretical formalism of Y. N. Qiu etal.[4,5], H. D Sun etal.[2] and S. B. Healy etal.[26], we have studied quantum well intermixing of GaInNAs/GaAs structure. We have evaluated Gallium concentration profile of GaInNAs along the growth direction on different diffusion lengths L_d. The

evaluation is performed with the help of Fick's law[12] and BAC model[24] with Luttinger-Kohn Hamiltonian[25]. The energy band gap of ternary alloy was calculated with the help of work done by C. S. Choules etal.[20] and I. Vurgaftman etal.[21]. The temperature dependence of the band gaps of binary materials were calculated using the empirical Vashni equation[22,23]. The in-plane strain of GaInNAs/GaAs quantum well as a function of growth axis z(m) for different values of diffusion length L_d were calculated by including a spin-orbit band into the calculation of valence band structure taking materials parameters into account. The parameters are effective mass, Luttinger parameters, the conduction band hydrostatic deformation potential, valance band hydrostatic deformation potential, shear deformation potential and elastic constants C_{11} and C_{12}. It has also been assumed that the strain layer semiconductor is grown on (0 0 1)-oriented substrate and only the biaxial strain exists.

In table T1, we have shown the evaluated results of Ga-concentration of GaInNAs along the growth direction z(m) for different values of diffusion length L_d. Our theoretically obtained results show that the concentration profile increase and decrease with z for each diffusion length L_d starting with L_d =0nm, 0.5nm, 1.0nm and 2.0nm respectively. The value of z is taken from -2<z<2. Our results indicate that with the increase of diffusion length L_d, the Gallium element in the barrier penetrates further into the quantum well which makes the gradual change of element concentration between the barrier and quantum well.

Table T1: An evaluated result of Ga concentration profile of GaInNAs along the growth direction z with different diffusion lengths L_d

Growth axis Z(m)x10^{-8}	← Ga concentration profile →			
	L_d =0	L_d =0.5nm	L_d =1.0nm	L_d =2.0nm
-2.00	1.087	0.952	0.852	0.786
-1.70	0.965	0.786	0.714	0.692
-1.50	0.902	0.679	0.609	0.599
-1.20	0.854	0.523	0.478	0.427
-1.00	0.738	0.478	0.386	0.339
-0.70	0.622	0.325	0.284	0.216
-0.50	0.589	0.227	0.176	0.125
0.00	0.478	0.126	0.108	0.097
0.50	0.398	0.149	0.157	0.184
0.70	0.522	0.296	0.256	0.297
1.00	0.698	0.384	0.367	0.385
1.20	0.893	0.489	0.478	0.496
1.50	0.987	0.674	0.596	0.654
1.70	1.017	0.887	0.688	0.789
2.00	1.086	0.923	0.862	0.847

In table T2, we have presented the evaluated results of in-plane strain of GaInNAs/GaAs quantum well as a function of growth direction z(m) for different values of diffusion lengths of L_d. Our theoretically obtained results show that the strain change from zero to negative values as a function of z for all the diffusion length taken. The value of z is taken from -2 to 2. We repeated the calculation for other value of L_d but same trend is observed. Our analysis shows that the quaternary GaInNAs is less strained than the ternary GaInAs. This is because the lattice constant of GaN and InN are small. Our evaluation also indicate that due to compressive strain the hydrostatic component widen the band

gap and shear component enlarge the splitting between the heavy hole (HH) and light hole(LH) at band edge at k=0.

Table T2: An evaluated result of in-plane strain of GaInNAs/GaAs quantum well as a function of growth axis z(m)x10^{-8} for different values of diffusion lengths L_d

Growth axis Z(m)x10^{-8}	← In-plane compressive strain(%) →			
	L_d =0nm	L_d= 1.0nm	L_d =1.5nm	L_d =2.0nm
-2.0	0.000	0.000	0.000	0.000
-1.70	-0.052	-0.048	-0.037	-0.028
-1.50	-0.187	-0.123	-0.109	-0.096
-1.20	-0.324	-0.296	-0.253	-0.197
-1.00	-0.587	-0.497	-0.387	-0.275
-0.70	-0.692	-0.588	-0.479	-0.389
-0.50	-0.748	-0.655	-0.586	-0.465
0.00	-1.022	-0.897	-0.678	-0.587
0.50	-0.987	-0.734	-0.567	-0.492
0.70	-0.853	-0.654	-0.509	-0.392
1.00	-0.786	-0.583	-0.416	-0.306
1.20	-0.632	-0.495	-0.355	-0.234
1.50	-0.587	-0.387	-0.298	-0.188
1.70	-0.496	-0.296	-0.212	-0.125
2.00	-0.322	-0.205	-0.186	-0.098
2.10	-0.265	-0.178	-0.145	-0.067

In table T3, we have shown the evaluated results of intensity of normalized PL spectra of $Ga_{0.728}In_{0.272}N_{0.0114}As_{0.9886}$/GaAs structure as a function of photon energy (meV) with two samples as-grown and PECVD (Plasma enhanced chemical vapour deposition) technique. Our theoretically obtained results show that intensity of normalized PL spectra (arb. u) increase and decrease as a function of photon energy for both the grown samples. However the intensity of Pl spectra is low for PECVD sample compared to as-grown sample. Our theoretically evaluated results are in good agreement with the compositional analysis of SIMS (Secondary ion mass spectroscopy)[10].

In table T4, we have shown the analysed experimental results of energy shift (meV) as a function of annealing temperature (^{0}C) for PECVD grown sample. The annealing duration was kept about 180s. Our analysed results show that energy shift increase with annealing temperature. The increase becomes fast by increasing the annealing temperature further. The results were performed using PLE and SIMS analysis. The result is also an indication that the increase is due to increase of band gap structure in the QW structure due to inter-diffusion of In-Ga between GaINNAs QWs and GaAs barrier[27].

Table T3: An evaluated result of intensity of normalized PL spectra (arb. u) of $Ga_{0.728}In_{0.272}N_{0.0114}As_{0.9886}$/GaAs structure as a function of photon energy (eV), the evaluation are performed on two growth samples (i) as-grown (ii) PECVD(Plasma enhanced chemical vapour deposition) technique

Photon energy (eV)	← Normalized PL intensity(arb. u) →	
	As-grown sample	PECVD sample
0.90	0.253	0.186
0.95	o.289	0.267
1.00	0.304	0.298
1.05	0.459	0.435
1.10	0.678	0.589
1.15	0.866	0.796
1.20	1.998	0.822
1.25	1.187	0.986
1.30	1.103	0.763
1.35	0.876	0.622
1.40	0.702	0.518
1.45	0.639	0.437
1.50	0.542	0.355
1.55	0.464	0.248
1.60	0.358	0.189

Table T4: An experimental result of energy shift (meV) as a function of annealing temperature (^{0}C) for PECVD grown sample, the annealing duration was taken about 180s, the experiment was performed by group led by H D Sun etal[2].

Annealing temperature (^{0}C)	Energy shift (meV)
500	0.284
550	0.685
570	1.584
580	2.687
600	3.539
630	4.556
650	10.679
670	15.846
700	24.349
730	45.584
750	57.386
800	85.439
850	92.184
900	112.45
950	123.56

In table T5, we have shown the experimental analysed results of normalized PL intensity of $Ga_{0.728}In_{0.272}N_{0.0114}As_{0.9886}$/GaAs structure as a function of wavelength (nm) at different annealing temperature. The annealing duration was again kept about 180s. Results were performed on PECVD grown sample for three different annealing temperatures 800^0C, 700^0C and 650^0C respectively. The analysed results show that the PL intensity increases with wavelength attain maximum peak value and then decrease. The same trend is observed for all the annealing temperatures.

Table T5: An experimental result of normalized PL intensity (arb. u) of $Ga_{0.728}In_{0.272}N_{0.0114}As_{0.9886}$/GaAs structure as a function of wavelength (nm) at different annealed temperatures, the annealing duration was about 180s, results were performed on PECVD grown sample

Wavelength (nm)	← PL intensity(arb. u) →		
	T=800(^{0}C)	T=700(^{0}C)	T=650(^{0}C)
1000	3.528	2.586	1.989
1050	4.867	4.321	2.764
1100	5.324	4.898	3.967
1150	6.897	5.764	4.863
1200	12.543	9.345	8.563
1250	15.469	11.694	9.056
1300	12.867	10.453	7.899
1350	11.232	9.246	6.894
1400	9.467	7.869	4.765
1450	7.249	5.342	3.158
1500	4.338	3.168	2.245
1550	2.167	1.085	1.006
1600	1.086	0.0876	0.759

In table T6, we have presented the experimental analysed results of energy shift (meV) of GaInNAs/GaAs structure as a function of annealing temperature with some fixed value of N-concentration. In this case also, the experimental results were performed by PECVD grown sample. The analysed results show that the energy shift increases as a function of annealing temperature for all the N-concentrations taken. The energy shift is large for N=0.5% and small for N=1.14%. This type of behaviour provides a support of the fact that the QWI originates from the inter-diffusion of In-Ga rather than N-As. All the experimental analysed results are in good agreement with the other theoretical workers[28-30]. There is some recent works[31-43] which also reveals the similar facts.

Table T6: An experimental result of dependence of PL energy shift (meV) as a function of annealing temperature (^{0}C) for different N contents (%) for GaInNAs/GaAs structure, results were performed on PECVS-$Si0_2$ capped sample

Annealing temperature(^{0}C)	← Energy shift (meV) →		
	N= 0.5%	N=0.85%	N=1.14%
450	0.879	0.322	0.287
500	1.584	0.479	0.345
550	2.285	1.986	0.979
600	7.489	6.328	5.275
650	10.905	9.064	7.544
700	16.675	14.225	9.865
750	22.248	19.584	12.432
800	32.296	28.765	18.884
850	44.675	38.955	27.906
900	57.846	55.186	50.557
950	68.438	64.378	64.986
1000	89.342	86.458	80.554
1050	132.78	108.546	98.448
1100	145.56	115.157	110.245

CONCLUSION

From the above theoretical investigations and analysis, we have come across the following conclusions:

- Our evaluated results of Ga-concentration profile along the growth axis z for different values of diffusion lengths L_d show that the concentration profile increase and decrease with z for each value of diffusion length. The results also indicate that with the increase of diffusion length, the Gallium element in the barrier penetrates further into the quantum well which makes the gradual change of the element concentration between the barrier and quantum well
- Our evaluated results of in-plane strain of GaInNAs/GaAs structure as a function of growth direction z for different values of diffusion length show that the strain change from zero to negative values foe all the diffusion lengths taken. This result indicates that the quaternary GaInNAs is less strained than the ternary GaInAs .This is because the lattice constants of GaN and InN are small. The evaluation also confirms that due to compressive strain the hydrostatic component widen the band gap and the shear component enlarge the splitting between heavy hole (HH) and light hole (LH) at band-edge at k=0.
- Our theoretically obtained results of intensity of normalized PL-spectra as a function of photon energy of GaInNAs/GaAs structure for two grown samples as-grown and PECVD grown sample show that the PL-intensity increase and decrease with photon energy. Our obtained results are in good agreement with the compositional analysis of SIMS.

- We have analysed the experimental results performed by the group led by H. D. Sun etal regarding the energy shift as a function of annealing temperature and energy shift for different N-concentrations. Our analysed results show that PL energy shift increase with decrease of N –concentration. This finding not only rules out the possible mechanism of N-As inter-diffusion but also demonstrates the alloy stability of GaInNAs due to strong bound of In-N. Our all experimental analysed results are in god agreement with the other theoretical workers.
- The entire evaluation is based on Fick's law and BAC model with Luttinger-Kohn Hamiltonian. The validity of the model has been confirmed by the excellent agreement with PLE data and SIMS results. The obtained results will be quite useful in the design of integrated photonic devices based on GaInNAs/GaAs material.

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