Study of interdiffusion in GaInNAs/GaAs quantum well structure emitting at 1.3 μm by eight-band $k\cdot p$ method

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The interdiffusion effect of GaInNAs/GaAs single quantum well (QW) has been investigated with the eight-band $k\cdot p$ method. The as-grown 64-Å $\text{Ga}_{0.64}\text{In}_{0.36}\text{N}_{0.017}\text{As}_{0.983}/250\text{-Å GaAs}$ QW is experimentally determined to emit at 1.27 μm in the literature. The compositional profile of the QW after interdiffusion is modeled by an error function distribution. Varying the diffusion length, the effects of interdiffusion on the unstrained band gap, in-plane strain, and confinement profiles are studied. The curve of the ground-state transition (C1-HH1) energy dependence on the interdiffusion length is obtained. Our work shows that the interdiffusion effect on the strain can greatly change the confinement profile of the lighthole (LH), which is confined in the GaAs layer, not in the GaInNAs layer. From the transition energy curve, a blueshift of 51 meV is derived. This interdiffusion mechanism can be utilized in the tuning of the laser operation wavelength. © 2005 American Institute of Physics. [DOI: 10.1063/1.1899226]

I. INTRODUCTION

In recent years, a number of studies have been carried out on GaInNAs grown on GaAs substrate due to their potential applications in 1.3- and 1.55- μm optical fiber communication.^{1–5} Compared with the widely used GaInPAs/InP quantum well (QW) systems, a small amount of nitrogen introduced into GaInAs can greatly reduce the band gap, which leads to a larger conduction-band offset between GaInNAs and GaAs. The mature AlGaAs/GaAs Bragg mirrors with high refractive index contrast can be directly used to fabricate vertical cavity surface-emitting laser (VCSEL). Meanwhile, due to the smaller lattice constant of GaN, less strain exists in GaInNAs/GaAs QWs.⁶

However, the performance of GaInNAs/GaAs lasers suffers from the poor crystal quality of GaInNAs, because of the incorporation of nitrogen.^{7,8} Nevertheless, the material quality and the optical properties of the QW can be improved greatly by rapid thermal annealing (RTA), which causes the constituent atoms to diffuse. The interdiffusion process can change the distribution of the constituent atoms across the interface of the QW, which in turn changes the band structure of the QW and leads to the blueshift of the emission wavelength.⁹

A theoretical study on the interdiffusion effect of GaInNAs/GaAs QW was reported by Chan *et al.*^{9,10} They used a parabolic band model and a four-band Pikus–Bir model for the conduction and valence band, respectively. In this work, a more realistic eight-band $k\cdot p$ method¹¹ is used to investigate the interdiffusion mechanism of GaInNAs/GaAs QW.

II. CALCULATION METHOD

A. Effects of interdiffusion

Two types of interdiffusion are possible in GaInNAs/GaAs QW: (1) the interdiffusion between In and

Ga atoms and (2) the interdiffusion between N and As atoms.^{7,12} However, recently Sun *et al.* discovered that the N-As interdiffusion mechanism is ruled out during thermal annealing due to the strong In–N bond.¹² Hence in our present work, we exclude the N-As sublattice diffusion and only consider the diffusion between In and Ga atoms. We then consider a single QW with undoped $\text{Ga}_{1-x}\text{In}_x\text{N}_{1-y}\text{As}_y$ grown on GaAs substrate and set x' and $1-x'$ as the composition of In and Ga atoms after In–Ga interdiffusion, respectively. The interdiffusion of In and Ga atoms is characterized by a diffusion length L_d ,¹³ which is equal to $(Dt)^{1/2}$, with the diffusion time t and the diffusion coefficient D . The In composition after interdiffusion is defined as⁹

$$x'(z) = \frac{x}{2} \left[\text{erf} \left(\frac{L_z + 2z}{4L_d} \right) + \text{erf} \left(\frac{L_z - 2z}{4L_d} \right) \right], \quad (1)$$

where z is the length along the growth direction, x is the as-grown composition of indium, and L_z is the QW width before interdiffusion. Consequently, all the QW parameters related to the In concentration will vary accordingly, which first causes the variation of strain and subsequently affects the subband energy distribution across the QW.

B. Interdiffusion effects on strain

If the QW layer thickness is within the critical thickness range, the strain is twofold: a biaxial hydrostatic strain along two perpendicular directions in the interfacial plane, which is called the in-plane strain, and a uniaxial shear strain along the growth direction, which is perpendicular to the interfacial plane.¹⁴ Assuming that the growth direction z is along $\langle 001 \rangle$, then for GaInNAs/GaAs QW system after interdiffusion, the in-plane strain $\varepsilon(x')$ is given by¹⁴

TABLE I. Parameters for binary compounds used in the calculation.

	GaAs ^a	InAs ^a	GaN ^b	InN ^b
Lattice constant a_0 (Å)	5.653 3	6.058 4	4.50	4.98
Spin-orbit splitting energy Δ_0 (meV)	341	390	17	5
Optical matrix parameter E_p (eV)	28.8	21.5	25.0	17.2
Deformation potential constant a_c (eV)	-7.17	-5.08	-6.17	-2.65
Deformation potential constant a_v (eV)	1.16	1.00	0.69	0.7
Shear deformation potential b (eV)	-2.0	-1.8	-2.0	-1.2
Elastic constant c_{11} (Gpa)	122.1	83.29	293	187
Elastic constant c_{12} (Gpa)	56.6	45.26	159	125
Luttinger parameter γ_1	6.98	20.0	2.70	3.72
Luttinger parameter γ_2	2.06	8.5	0.76	1.26
Luttinger parameter γ_3	2.93	9.2	1.11	1.63
Unstrained band-gap energy $E_g(T=300\text{ K})$ (eV)	1.422	0.354	3.24	0.756

^aReference 18.^bReference 19.

$$\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon(x') = \frac{a_b(x') - a_w(x')}{a_w(x')},$$

$$\varepsilon_{zz} = -2[c_{12}(x')/c_{11}(x')]\varepsilon(x'), \quad (2)$$

$$\varepsilon_{xy} = \varepsilon_{yz} = \varepsilon_{zx} = 0,$$

where $c_{11}(x')$ and $c_{12}(x')$ are the elastic stiffness constants and $a_b(x')$ and $a_w(x')$ are the lattice constants for the barrier and well material, respectively. When the strain of GaInNAs/GaAs QW is compressive, $\varepsilon(x')$ is negative.

Taking the interdiffusion effects on strain into account, the expressions for the electron and hole band-edge energy can be written as

$$E_n^s(x') = E_n(x') - \Delta E_n(x') \pm Q_\varepsilon(x'), \quad (3)$$

where n is for the respective band (using c for the conduction band, hh for the heavy-hole (HH) band and lh for the LH band), $E_n^s(x')$ represents the strained band-edge energy, $E_n(x')$ is the unstrained band-edge energy, and $\Delta E_n(x')$ is the change of the respective band edge due to the hydrostatic strain. For the conduction band, we have

$$\begin{aligned} \Delta E_c(x') &= a_c(x')(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) \\ &= 2a_c(x')\left(1 - \frac{c_{12}(x')}{c_{11}(x')}\right)\varepsilon(x'), \end{aligned} \quad (4)$$

where $a_c(x')$ is the hydrostatic deformation potential in the conduction band. For the HH band, we have

$$\begin{aligned} \Delta E_{hh}(x') &= -a_v(x')(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) \\ &= -2a_v(x')\left(1 - \frac{c_{12}(x')}{c_{11}(x')}\right)\varepsilon(x'), \end{aligned} \quad (5)$$

where $a_v(x')$ is the hydrostatic deformation potential in the valence band. For the LH band, we have

$$\Delta E_{lh}(x') = \Delta E_{hh}(x'). \quad (6)$$

Due to the shear strain, the degeneracy of the HH and LH band will be violated. The HH band is shifting upward, while the LH band is shifting downward for the compressive strain

case. The absolute energies of both shifting are the same $|Q_\varepsilon(x')|$ and $Q_\varepsilon(x')$ can be written as

$$Q_\varepsilon(x') = -b(x')\left(1 + 2\frac{c_{12}(x')}{c_{11}(x')}\right)\varepsilon(x'), \quad (7)$$

where $b(x')$ is the shear deformation potential. In Eq. (3), for the conduction band $Q_\varepsilon(x')$ is zero, while the sign before $Q_\varepsilon(x')$ is “+” and “-” for the LH and HH band, respectively.

C. Electronic band structure calculation

The band structure of the QW can be obtained by solving the equation below:

$$H\Psi = E\Psi, \quad (8)$$

where Ψ is the total wave function. In the eight-band $k \cdot p$ method, at a given $k_{\parallel}$, it can be written as¹⁵

$$\Psi_{\mathbf{k}_{\parallel}}(z) = \sum_{i=1}^8 e^{i\mathbf{k}_{\parallel} \cdot \mathbf{r}_{\parallel}} \phi_i(z) u_i(\mathbf{r}), \quad (9)$$

where $\mathbf{k}_{\parallel} = k_x \bar{i} + k_y \bar{j}$, $\mathbf{r}_{\parallel} = x\bar{i} + y\bar{j}$, $\mathbf{r} = x\bar{i} + y\bar{j} + z\bar{k}$, ϕ_i is the eight-dimensional envelope wave function for the QWs, and u_i is the periodic Bloch wave function. The detailed solution of Eq. (8) is described in our previous work¹⁶ (the Hamiltonian matrix is listed in Appendix A).

III. RESULTS AND DISCUSSION

In this work, a 64-Å Ga_{0.64}In_{0.36}N_{0.017}As_{0.983}/250-Å GaAs QW structure is considered, similar to the structure investigated in Ref. 17 to achieve 1.3-μm emission. We further assume that the band offset ratio of the conduction band is 75% and the temperature is taken to be 300 K in our study. The material parameters for binary semiconductors can be found in Table I. (The detailed parameter calculations for GaInNAs are listed in Appendix B).

Figure 1 shows the dependence on diffusion length of the electron, HH, and LH confinement profiles of the 64-Å Ga_{0.64}In_{0.36}N_{0.017}As_{0.983}/250-Å GaAs strained QW structure along the growth axis with diffusion length varying from 0 to 1.5 nm in steps of 0.5 nm. The origin is taken to be the

FIG. 1. Dependence of electron, heavy-hole, and light-hole confinement potential for 64-Å $\text{Ga}_{0.64}\text{In}_{0.36}\text{N}_{0.017}\text{As}_{0.983}/250\text{-}\text{\AA}$ GaAs QW on diffusion length. $L_d=0$ nm (solid line), $L_d=0.5$ nm (dashed line), $L_d=1$ nm (dotted line), and $L_d=1.5$ nm (dashed dotted line), with well center at $z=0$.

valence band maximum after strain. The confinement profiles change gradually near the interface due to the In-Ga interdiffusion.

The profile of the unstrained band gap $E_g(x')$ after In-Ga interdiffusion is shown in Fig. 2(a). The In atoms in the well diffuse into the GaAs barrier and the Ga atoms diffuse into the well layer, so that a new GaInNAs/GaInAs graded interface appears (the As-N interdiffusion is omitted). Considering that the bulk band gap of GaAs is greater than that of InAs, as the interdiffusion proceeds, the unstrained band gap of GaInNAs gradually increases with z approaching the interface in the well region, while that of GaInAs decreases with z approaching the interface in the barrier region. The room-temperature strained band gap $E_g^s(x')$ is calculated as

$$E_g^s(x') = E_g(x') + \Delta E_c(x') + \Delta E_{hh}(x') + Q_\varepsilon(x'). \quad (10)$$

To illustrate how the unstrained band gap is modified by strain, we define $E_{gs}(x')$ as

$$E_{gs}(x') = \Delta E_c(x') + \Delta E_{hh}(x') + Q_\varepsilon(x'). \quad (11)$$

Thereby, Eq. (10) can be rewritten as

$$E_g^s(x') = E_g(x') + E_{gs}(x') \quad (12)$$

the profiles of $E_{gs}(x')$ and $E_g^s(x')$ with interdiffusion are shown in Figs. 2(b) and 2(c), respectively. As the figure indicates, for the numerical case $L_d=1.5$ nm, at the well center ($z=0$ nm), the corresponding ΔE_c , ΔE_{hh} , and Q_ε are 125, 21,

FIG. 2. Dependence of (a) bulk band-gap energy E_g profile, (b) the change of the band gap due to strain E_{gs} , and (c) strained band-gap energy E_g^s profile for 64-Å $\text{Ga}_{0.64}\text{In}_{0.36}\text{N}_{0.017}\text{As}_{0.983}/250\text{-}\text{\AA}$ GaAs QW on diffusion length. $L_d=0$ nm (solid line), $L_d=0.5$ nm (dashed line), $L_d=1$ nm (dotted line), and $L_d=1.5$ nm (dashed dotted line), with well center at $z=0$.

FIG. 3. Dependence of (a) heavy-hole band-edge profile and (b) $2 \times Q_\varepsilon$ profile for 64-Å $\text{Ga}_{0.64}\text{In}_{0.36}\text{N}_{0.017}\text{As}_{0.983}/250\text{-}\text{\AA}$ GaAs QW on diffusion length. $L_d=0$ nm (solid line), $L_d=0.5$ nm (dashed line), $L_d=1$ nm (dotted line), and $L_d=1.5$ nm (dashed dotted line), with well center at $z=0$.

and -71 meV, respectively, resulting in $E_{gs}=75$ meV; while at a point in the well region near the interface ($z=3.1$ nm), the corresponding ΔE_c , ΔE_{hh} , and Q_ε are 69, 12, and -38 meV, respectively, leading to $E_{gs}=43$ meV. Thereby, $|E_{gs}(x'(z=3.1)) - E_{gs}(x'(z=0))| = 32$ meV, while $|E_g(x'(z=3.1)) - E_g(x'(z=0))| = 126$ meV. It shows that the strain produced in the diffused QW reduces the depth of the band-gap profile in the well, as depicted in Fig. 2(c) with comparison to Fig. 2(a). The same explanation applies to the profile of the band gap after strain in the barrier. We define the band offsets of the conduction band and valence band after strain as $E_{c_offset}^s(x')$ and $E_{v_offset}^s(x')$, respectively, which satisfy

$$E_{c_offset}^s(x') + E_{v_offset}^s(x') + E_g^s(x') = E_g(\text{GaAs}(300\text{ K}))$$

$$\frac{E_{c_offset}^s(x')}{E_{v_offset}^s(x')} = \frac{75\%}{25\%} = 3. \quad (13)$$

In going from the well center to the interface, $E_g^s(x')$ increases, so that the potential of the electron profile increases, while that of the HH profile decreases. The converse holds for the case along the direction from the barrier to the interface, as shown in Fig. 1. However, for the case of the LH confinement profile, we observe an interesting structure. The as-grown GaAs valence band actually lies above the as-grown GaInNAs LH band, forming a potential barrier in the GaInNAs layer and a potential well in the GaAs layer, which is contrary to the normal case. This type of the LH band configuration is verified to be possible for GaInAs/GaAs (Ref. 20). Figure 1 also tells us that the diffused LH profile is reversed from the diffused HH profile, in contrast to the result of Ref. 9. From Eq. (3), we derive the relationship between $E_{hh}^s(x')$ and $E_{lh}^s(x')$ as

$$E_{lh}^s(x') = E_{hh}^s(x') + 2Q_\varepsilon(x'). \quad (14)$$

The profiles of $E_{hh}^s(x')$ and $2Q_\varepsilon(x')$ are shown in Figs. 3(a) and 3(b), respectively. As the figures indicate, the HH band edge of the as-grown profile lies about 120 meV higher above the valence band edge (VBE) of GaAs, while the profile of $2Q_\varepsilon(x')$ in the well region lies about 167 meV lower than the VBE of GaAs. Consequently, it causes the as-grown LH band edge to be pushed below the VBE of GaAs and form a weakly type-II structure for the LH band profile. Con-

FIG. 4. Dependence of C1-HH1 transition energy for 64-Å $\text{Ga}_{0.64}\text{In}_{0.36}\text{N}_{0.017}\text{As}_{0.983}/250$ -Å GaAs QW on diffusion length. $L_d=0, 0.5, 1$, and 1.5 nm.

sidering the interdiffusion effect, for the case $L_d=1.5$ nm, at the well center ($z=0$ nm), E_{hh}^s and $2Q_e$ are -9 and -142 meV, respectively. It follows that $E_{lh}^s=-151$ meV, which is below the VBE of GaAs (-122 meV). As z approaches the interface in the well region ($z=3.1$ nm), E_{hh}^s and $2Q_e$ are -33 and -75 meV, respectively, leading to $E_{lh}^s=-108$ meV, which is above the VBE of GaAs. It reveals that the increase of $2Q_e(x')$ is faster than the reduction of $E_{lh}^s(x')$ in the well region. The same observation applies to the case in the barrier region. As can be seen from observations given above, the shear strain produced in the disordered QW structure combining with a small valence band (HH band) offset forces the LH confinement profile from being reversed from the HH confinement profile. This explains the LH band curves of Fig. 1.

The variation of C1-HH1 transition energy with interdiffusion for a 64-Å $\text{Ga}_{0.64}\text{In}_{0.36}\text{N}_{0.017}\text{As}_{0.983}/250$ -Å GaAs QW structure is shown in Fig. 4. As the interdiffusion proceeds, a strong blueshift is obtained. The emission wavelength of the as-grown structure is $1.29 \mu\text{m}$ (961 meV) calculated by the eight-band $k \cdot p$ method, which is in good agreement with the

experimental result given in Ref. 17 ($1.27 \mu\text{m}$). As L_d increases to 1.5 nm, the wavelength can be shifted to $1.225 \mu\text{m}$ (1012 meV).

IV. CONCLUSION

The interdiffusion of a compressively strained 64-Å $\text{Ga}_{0.64}\text{In}_{0.36}\text{N}_{0.017}\text{As}_{0.983}/250$ -Å GaAs QW has been studied by using an error function to model the compositional profiles. Ga-In interdiffusion causes the formation of a GaInNAs/GaInAs interface, while the N-As interdiffusion is ruled out by recent research. As diffusion proceeds, it can result in a wider effective well width and a lower effective barrier of the confinement profiles. We would like to note that the LH confinement profile is reversed from the HH confinement profile, indicating that the interdiffusion-dependent strain effects can modify some band edges significantly. The ground-state (C1-HH1) transition energy calculated by the eight-band $k \cdot p$ method is 961 meV, which corresponds to an emission wavelength of $1.29 \mu\text{m}$ and agrees very well with the reported $1.27 \mu\text{m}$. Finally the dependence of the C1-HH1 transition energy on the diffusion length is obtained, which shows a 51-meV blueshift as diffusion length increases to 1.5 nm.

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APPENDIX A: 8×8 $K \cdot P$ HAMILTONIAN MATRIX

In the presence of strain, the Hamiltonian H consists of three parts: 8×8 nonstrain Hamiltonian H_k , 8×8 strain Hamiltonian H_s , and the band offset potential $V(z)$. The strain-free Hamiltonian H_k is extracted from Ref. 11

$$H_k = \begin{bmatrix} C & 0 & \frac{-1}{\sqrt{2}}P^+ & \sqrt{\frac{2}{3}}P^z & \frac{1}{\sqrt{6}}P^- & 0 & \frac{1}{\sqrt{3}}P^z & \frac{1}{\sqrt{3}}P^- \\ 0 & C & 0 & \frac{-1}{\sqrt{6}}P^+ & \sqrt{\frac{2}{3}}P^z & \frac{1}{\sqrt{2}}P^- & \frac{1}{\sqrt{3}}P^+ & \frac{-1}{\sqrt{3}}P^z \\ \text{c.c.} & 0 & H & \alpha & \beta & 0 & \frac{1}{\sqrt{2}}\alpha & \frac{1}{\sqrt{2}}\beta \\ \text{c.c.} & \text{c.c.} & \text{c.c.} & L & 0 & \beta & -\sqrt{2}D & -\sqrt{\frac{3}{2}}\alpha \\ \text{c.c.} & \text{c.c.} & \text{c.c.} & 0 & L & -\alpha & -\sqrt{\frac{3}{2}}\alpha^* & \sqrt{2}D \\ 0 & \text{c.c.} & 0 & \text{c.c.} & \text{c.c.} & H & -\sqrt{2}\beta^* & \frac{1}{\sqrt{2}}\alpha^* \\ \text{c.c.} & \text{c.c.} & \text{c.c.} & \text{c.c.} & \text{c.c.} & \text{c.c.} & S & 0 \\ \text{c.c.} & \text{c.c.} & \text{c.c.} & \text{c.c.} & \text{c.c.} & \text{c.c.} & 0 & S \end{bmatrix}, \quad (\text{A1})$$

where

$$\begin{aligned}
 C &= E_g + \frac{\hbar^2}{2m_0}(k_x^2 + k_y^2 + k_z^2)\tilde{\gamma}_C, \\
 H &= \frac{\hbar^2}{2m_0}[-(k_x^2 + k_y^2)(\tilde{\gamma}_1 + \tilde{\gamma}_2) - k_z^2(\tilde{\gamma}_1 - 2\tilde{\gamma}_2)], \\
 L &= \frac{\hbar^2}{2m_0}[-(k_x^2 + k_y^2)(\tilde{\gamma}_1 - \tilde{\gamma}_2) - k_z^2(\tilde{\gamma}_1 + 2\tilde{\gamma}_2)], \\
 S &= \frac{\hbar^2}{2m_0}[-(k_x^2 + k_y^2 + k_z^2)\tilde{\gamma}_1] - \Delta_0, \\
 P^+ &= P(k_x + ik_y), \\
 P^- &= P(k_x - ik_y), \\
 P^z &= Pk_z, \\
 \alpha &= \frac{\hbar^2}{2m_0}2\sqrt{3}[k_z(k_x - ik_y)\tilde{\gamma}_3], \\
 \beta &= \frac{\hbar^2}{2m_0}\sqrt{3}[(k_x^2 - k_y^2)\tilde{\gamma}_2 - 2ik_xk_y\tilde{\gamma}_3], \\
 D &= \frac{\hbar^2}{2m_0}[2k_z^2 - (k_x^2 + k_y^2)]\tilde{\gamma}_2, \\
 \tilde{\gamma}_c &= \frac{1}{m_e^*} - \frac{E_P}{3}\left(\frac{2}{E_g^0} + \frac{1}{E_g^0 + \Delta_0}\right), \\
 \tilde{\gamma}_1 &= \gamma_1 - \frac{E_P}{3E_g^0}, \\
 \tilde{\gamma}_2 &= \gamma_2 - \frac{E_P}{6E_g^0}, \\
 \tilde{\gamma}_3 &= \gamma_3 - \frac{E_P}{6E_g^0},
 \end{aligned} \tag{A2}$$

and the momentum matrix element P satisfies²¹

$$E_P = \frac{2m_0}{\hbar^2}P^2. \tag{A3}$$

E_g^0 is the unstrained band gap of the bulk material and other parameters in Eqs. (A2) and (A3) are defined as usual. Their values for the parental binary compounds are given in Table I. The strain Hamiltonian H_s can be derived by simply substituting $\varepsilon_{\alpha\beta}$ into $k_\alpha k_\beta$ with $\alpha, \beta = x, y, z$.

APPENDIX B: PARAMETER CALCULATION FOR GAINNAS

Except for the band-gap energy and electron effective mass, most parameters for $\text{Ga}_{1-x'}\text{In}_{x'}\text{N}_{1-y}\text{As}_y$ materials are obtained using a linear interpolation between the parameters of the relevant binary compounds, including the interdiffusion effect, which can be expressed as¹⁴

$$\begin{aligned}
 P(\text{Ga}_{1-x'}\text{In}_{x'}\text{N}_{1-y}\text{As}_y) &= P(\text{GaAs})(1-x')y + P(\text{InAs})x'y \\
 &+ P(\text{GaN})(1-x')(1-y) \\
 &+ P(\text{InN})x'(1-y).
 \end{aligned} \tag{B1}$$

The band-gap energy, considering temperature variation, is calculated by the band anticrossing (BAC) model and taking parameter definitions in Ref. 22

$$\begin{aligned}
 E_g(\text{Ga}_{1-x'}\text{In}_{x'}\text{N}_{1-y}\text{As}_y) &= \frac{1}{2}[E_g(\text{Ga}_{1-x'}\text{In}_{x'}\text{As}) + E^N \\
 &- \sqrt{[E_g(\text{Ga}_{1-x'}\text{In}_{x'}\text{As}) - E^N]^2 + 4V^2(1-y)}],
 \end{aligned} \tag{B2}$$

where $E^N = 1.65 - 0.31x'$ and $V = 2.4 - 0.65x'$. $E_g(\text{Ga}_{1-x'}\text{In}_{x'}\text{As})$ is calculated by¹⁸

$$\begin{aligned}
 E_g(\text{Ga}_{1-x'}\text{In}_{x'}\text{As}) &= (1-x')E_g(\text{GaAs}) + x'E_g(\text{InAs}) \\
 &- x'(1-x')C,
 \end{aligned} \tag{B3}$$

where C is the bowing parameter, which is assumed to be 0.32. The electron effective mass is given by²³

$$\begin{aligned}
 m_e(\text{Ga}_{1-x'}\text{In}_{x'}\text{N}_y\text{As}_{1-y}) &= m_e(\text{Ga}_{1-x'}\text{In}_{x'}\text{As}) \\
 &+ 18.1667m_0\Delta e(x', y).
 \end{aligned} \tag{B4}$$

$\Delta e(x', y) = e(x', y) - e(x', 0)$ is the difference of the in-plane strain between $\text{Ga}_{1-x'}\text{In}_{x'}\text{N}_{1-y}\text{As}_y/\text{GaAs}$ QW and $\text{Ga}_{1-x'}\text{In}_{x'}\text{As}/\text{GaAs}$ QW, which can be calculated by

$$e(x', y) = \frac{a(\text{GaAs}) - a(\text{Ga}_{1-x'}\text{In}_{x'}\text{N}_{1-y}\text{As}_y)}{a(\text{Ga}_{1-x'}\text{In}_{x'}\text{N}_{1-y}\text{As}_y)}, \tag{B5}$$

$$e(x', 0) = \frac{a(\text{GaAs}) - a(\text{Ga}_{1-x'}\text{In}_{x'}\text{As})}{a(\text{Ga}_{1-x'}\text{In}_{x'}\text{As})}, \tag{B6}$$

respectively.

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