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ANALYSIS OF THREE TYPES OF INTERDIFFUSION PROCESS IN INGAAS/INP QUANTUM-WELL AND THEIR DEVICES IMPLICATIONS

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ABSTRACT

The optical properties of $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{InP}$ single quantum well (QW) (with an as-grown well width of 60\AA structures) interdiffused with different cation and anion interdiffusion rates have been theoretically analyzed for applications in optoelectronics. The interdiffusion of InGaAs/InP QW structures is complicated as interdiffusion can occur for either (i) only group-III (In,Ga), (ii) group-V (As,P), or (iii) both group-III and group-V sublattices. Depending on the resulting composition profiles, the shifts (blue or red) of the transition energies can be tuned to wavelengths between $1.3\mu\text{m}$ to $1.55\mu\text{m}$ for device applications. The results show that the control of the rates of cation and anion interdiffusion offers interesting possibilities for designing optoelectronic devices such as modulators and lasers.

INTRODUCTION

Currently InGaAs/InP quantum-well (QW) structures are actively studied for the fabrication of a variety of optoelectronic devices, such as modulators, detectors, waveguides, and lasers, for operation in the $1.3\mu\text{m}$ - $1.55\mu\text{m}$ wavelength region¹. By exploiting the strain effects on the band-gap, the bandstructure of the device can be engineered to optimize the device characteristics. Apart from this, interdiffusion of constituent atoms, the rate of which depends on lattice distortion, impurities, defects and the process temperature, is a versatile technique to modify the device bandstructure. Using this technique, the QW compositional profiles, the confinement potentials and the optical properties can be modified as a result of the diffusion of constituent atoms. The interdiffusion processes in InGaAs/InP QW system is more complex than those in $\text{AlGaAs}/\text{GaAs}$ and $\text{InGaAs}/\text{GaAs}$ because both group-III and group-V atoms can participate in the interdiffusion process. Although some theoretical² and experimental³ studies were undertaken on $(\text{In,Ga})(\text{As,P})/\text{InP}$ QWs, the mechanism of interdiffusion in these systems is not well understood. In order to predict the interdiffused compositional profiles, some hypotheses have to be made. The interdiffusion processes of group-III and group-V atoms are assumed to be independent and there are three categories of interdiffusion: (i) only group-III diffusion, (ii) only group-V diffusion, and (iii) both group-III and group-V diffusion. It has been reported that group-V atoms is more easily interdiffused than group-III atoms. Arsenic and phosphorus atoms begin to interdiffuse at about $500\text{ }^\circ\text{C}$ while group-III atoms are known to interdiffuse above $800\text{ }^\circ\text{C}$ ⁴. The control of diffusing atoms is determined by the impurities in the structure. It is thus important to understand the effects of interdiffusion on the optical characteristics of InGaAs/InP QWs for integration and optimization of devices. In this paper, we model the interdiffusion processes in an undoped InGaAs/InP single QW and study their effects on the optical properties.

MODEL FORMULATION

It is assumed that for diffusion processes (i) and (ii) the group-III and group-V interdiffusion processes can be modeled by two different diffusion lengths. The interdiffusion of group-III atoms is characterized by a diffusion length L_d^{III} , which is defined as $L_d^{III} = \sqrt{(D^{III}t)}$, where D^{III} is the diffusion coefficient of group-III atoms and t is the diffusion time; the interdiffusion of group-V atoms is characterized by the diffusion length L_d^V . The structure modeled here consists of an as-grown $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ square well with thickness 60\AA sandwiched between thick InP barriers. After intermixing, the concentration of the interdiffused atoms across the QW structure has an error function profile. For the group-III atoms, the In concentration after interdiffusion is described by

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

where L_z is the as-grown well width, z is the growth direction, and the QW is centered at $z=0$. For the group-V atoms, the As concentration after interdiffusion is given by

$$y_{\text{As}}(z) = \frac{y}{2} \left[\text{erf}\left(\frac{L_z + 2z}{4L_d^V}\right) + \text{erf}\left(\frac{L_z - 2z}{4L_d^V}\right) \right] \quad (2)$$

where $y=1$ is the As concentration of the as-grown structure. For diffusion of group V atoms only, Mukai *et al*⁴ studied in details the diffusion of group-V atoms in InGaAs/InP and found that the diffusion coefficients are different in the barrier and well layers and the concentration of group-V atoms is discontinuous across the interface. Here in the present work, we model the diffusion process (iii) using the two phase model described in Mukai *et al*.

In this paper, we consider the interdiffusion of $\text{In}_{0.53}\text{Ga}_{0.47}\text{As/InP}$ QW, in which the QW layer is lattice-matched to the barrier layers. After interdiffusion, the chemical compositions deviates from the lattice-matched condition leading to a non-uniform strain in the lattice. To calculate the electron and hole wave functions in QW, we use the effective mass theory. For most III-V semiconductors, it is a good approximation that the conduction and valence bands are decoupled. A parabolic band model and the Luttinger-Kohn- Hamiltonian with strain components are used for the conduction and valence bands respectively. The electron states near the conduction subband edge are assumed to be s-like and nondegenerate (excluding spin), while the hole states near the valence subband edge are p-like and four-fold degenerate (including spin). The envelope function scheme is adopted to describe the slowly varying (spatially extended) part of the wavefunction. The wavefunctions of the electron and hole subbands at the zone centre can be calculated separately by solving the one-dimensional Schrodinger-like equation as follows:

$$-\frac{\hbar^2}{2} \frac{d}{dz} \left[\frac{1}{m_{1r}^*(z)} \frac{d\psi_{rl}(z)}{dz} \right] + U_r(z) \cdot \psi_{rl}(z) = E_{rl} \psi_{rl}(z) \quad (3)$$

where $\psi_{rl}(z)$ is the wavefunction of the l^{th} subband for electrons($r=\text{cl}$) or holes ($r=\text{vl}$), respectively; $m_{1r}^*(z)$ is the corresponding carrier effective mass in the z direction; E_{rl} is the subband-edge energy. Equation (3) is solved numerically using a finite difference method with

the above confinement profile. For valence band structure, it is necessary to diagonalize the Luttinger-Kohn Hamiltonian with appropriate confinement potentials for heavy and light holes. The hole envelope functions depend on $k_{//}$ as a result of the mixing of the heavy and light hole bands. In this work, the effective Hamiltonian approach described in Chan⁵ is used to solve the Luttinger-Kohn Hamiltonian to obtain the valence subband structure.

The polarization dependent absorption coefficient and optical gain are calculated using the following equations, where the orientation of the polarization is also considered:

$$g(\omega) = \frac{e^2 M_b^2}{\pi \epsilon_0 n_R c_0 m_0^2 \omega L_z} \sum_{p,q} \int \left| \langle \Psi_{c_p} | \Psi_{v_q} \rangle \right|^2 L(E_p(k) - E_q(k) - \hbar\omega) [f^c(E_p(k)) - f^v(E_q(k))] dk \quad (4)$$

$$\alpha(\omega) = \frac{e^2 M_b^2}{\pi \epsilon_0 n_R c_0 m_0^2 \omega L_z} \sum_{p,q} \int \left| \langle \Psi_{c_p} | \Psi_{v_q} \rangle \right|^2 L(E_p(k) - E_q(k) - \hbar\omega) dk \quad (5)$$

where L_z is QW width, n_R is the refractive index, c_0 is the velocity of light in vacuum and ϵ_0 is the permittivity of free space; e and m_0 are the electron charge and rest mass respectively; $M_b^2 = (m_0^2 P^2 / 3\hbar) M^2(\theta)$ where P is given by Kane's model, and $M(\theta)$ is a factor due to the difference in orientation between the confined carrier in-plane wave vector and the optical polarization vector (represented by θ); k is the transverse wave vector in the direction parallel to the QW layer; E_p and E_q are the electron and hole subband energy respectively; ψ_c and ψ_v are the envelope wavefunctions for the electrons and holes respectively; L is the Lorentzian broadening factor with HWHM $\Gamma_b = 5\text{meV}$. The summation in (4) and (5) includes all the bound states in the conduction (p) and valence (q) bands. The Fermi functions, f^c and f^v , are solved numerically for the quasi-Fermi levels at a fixed carrier injection ($n^{2D} = 3 \times 10^{12} / \text{cm}^2$).

RESULTS AND DISCUSSIONS

In the present study, we consider a 60Å-thick undoped $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ single quantum well layer sandwiched between 300Å-thick InP barriers. All the parameters are determined by interpolating between the binary parameters at room temperature. A general parameter T for the quaternary material $\text{A}_x\text{B}_{1-x}\text{C}_y\text{D}_{1-y}$ can be related to the parameters of four binary compounds AC, AD, BC, and BD using the following interpolation formula

$$T(x,y) = (1-x)yT_{BC} + xyT_{AC} + x(1-y)T_{AD} + (1-x)(1-y)T_{BD} \quad (6)$$

The compositional dependence of bulk bandgap in eV is given by⁶

$$E_g(x,y) = 1.35 - 1.17y + 0.668(1-x) - 0.069(1-x)y + 0.18y^2 + 0.03(1-x)y^2 + 0.758(1-x)^2 - 0.322(1-x)^2y \quad (7)$$

while the spin-orbit splitting, in eV, is given by⁷

$$\Delta_0(x,y) = 0.34(1-x)y + 0.43xy + 0.1(1-x)(1-y) + 0.1x(1-y) \quad (8)$$

The conduction band offset Q_c of InGaAs/InP heterostructures is taken to be 0.6.

The optical gain results of interdiffused lattice-matched InGaAs/InP QW for different diffusion processes are shown in figure 1. In fig.1(a), we show the gain of QW with interdiffusion of only group III sublattice. The peak gain energy shifts to lower energies as interdiffusion proceeds and the peak gain magnitude increases with the degree of interdiffusion.

This is due to the deepening of the QW potential and the increase in confinement when the group-III atoms interdiffuse. The gain spectra of wells with interdiffusion of both group-III and group-V sublattices are shown in figure 1(b). The error function confinement profile of this kind of interdiffused QW shifts the peak of the gain spectrum to higher energies and reduces the peak height. Figure 1(c) shows the gain after interdiffusion of group V sublattice. It is noticed that the peak gain energy shift to higher energies when the well is interdiffused.

The absorption coefficients of interdiffused InGaAs/InP QWs calculated in the present study include the 1s heavy and light hole exciton transitions. The 1s bound exciton wavefunction is determined by a perturbative-variational method⁸, and the exciton envelope function is given by:

$$\psi_{1s}(\rho) = \frac{4\lambda}{\sqrt{2\pi a^*}} e^{-\frac{2\rho\lambda}{a^*}} \quad (9)$$

where $a^* = \frac{4\pi\epsilon\hbar^2}{\mu_e e^2}$ is the exciton Bohr radius, ρ is the relative distance between the electron and (heavy or light) hole in the quantum well along the transverse direction, which is denoted by // and is parallel to the quantum well layer. $\mu_{//}$ is the reduced effective mass in the transverse direction. ϵ is the static dielectric constant. The variational parameter λ is obtained by minimizing the following expression:

$$\iint dz_e dz_v |\Psi_{e1}(z_e)|^2 |\Psi_{v1}(z_v)|^2 \left\{ \frac{1}{4} a^* + z - \frac{1}{2} \pi z \left[H_1\left(\frac{4\lambda z}{a^*}\right) - N_1\left(\frac{4\lambda z}{a^*}\right) \right] \right\} \quad (10)$$

where z_e and z_v are the electron and hole positions, $z=|z_e-z_v|$, Ψ_{e1} , Ψ_{v1} are the electron and hole envelope wavefunctions, H_1 and N_1 are the Struve and Neumann functions of order 1, respectively. The binding energy E_b of the 1s bound exciton is obtained by the parameter λ and is defined by:

$$E_b = -4\lambda^2 R \quad (11)$$

where $R = \frac{\mu_e e^4}{32\pi^2 \epsilon^2 \hbar^2}$ is the Rydberg energy. The exciton absorption coefficient, $\alpha_{1s}(\omega)$, is given by:

$$\alpha_{1s}(\omega) = \frac{A\omega}{c_v n_R} |\Psi(\rho=0)|^2 \frac{\Gamma_b}{\pi(E_{exc} - \hbar\omega)^2 + \Gamma_b^2} \quad (12)$$

where $A = \frac{e^2 \hbar^2}{3\epsilon_v m_e^* E_{cv}^2 L_z} M_0 \langle \Psi_{e1} | \Psi_{v1} \rangle^2 \wp$, $E_{exc} = E_{c1} + E_{v1} + E_g + E_b$, and Γ_b is the exciton linewidth (half width half maximum) broadening factor. For the 1s exciton only $\rho=0$ is allowed and hence $\wp^{1E} = 3/2(\text{hh})$, $1/2(\text{lh})$ and $\wp^{TM} = 0(\text{hh})$, $2(\text{lh})$. The calculated exciton binding energies are shown in tables 1-3 as a function of the diffusion lengths.

Table 1 Exciton Binding Energies of interdiffused InGaAs/InP QW (Group III only)

Group-III diffusion length (Å)	$L_d=0$	$L_d=10$	$L_d=20$	$L_d=30$	$L_d=40$
HH Binding Energy (meV)	4.84	4.38	4.07	3.80	3.62
LH Binding Energy (meV)	5.92	5.33	4.91	4.57	4.34

Table 2 Exciton Binding Energies of interdiffused InGaAs/InP QW (Group III&V, $L_d^{\text{III}} = L_d^{\text{V}} = L_d$)

diffusion length (Å)	$L_d=0\text{Å}$	$L_d=10$	$L_d=20$	$L_d=30$	$L_d=40$
HH Binding Energy (meV)	4.84	5.98	6.33	6.62	6.71
LH Binding Energy (meV)	5.92	6.91	7.43	7.56	7.74

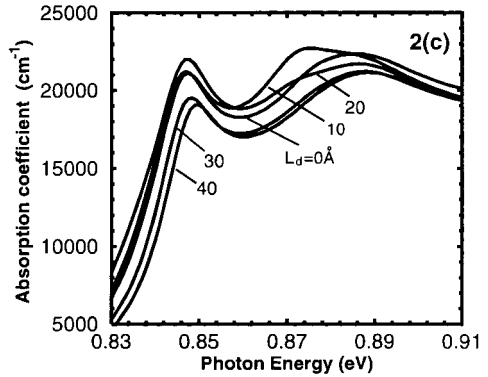
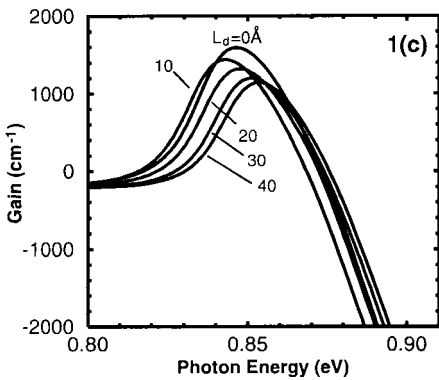
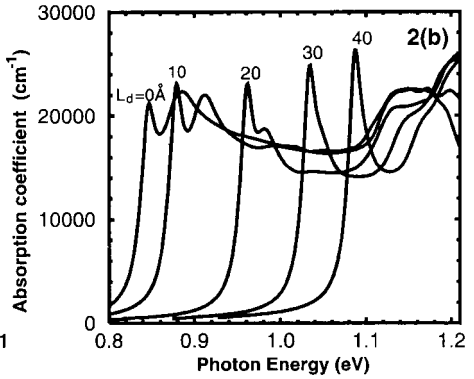
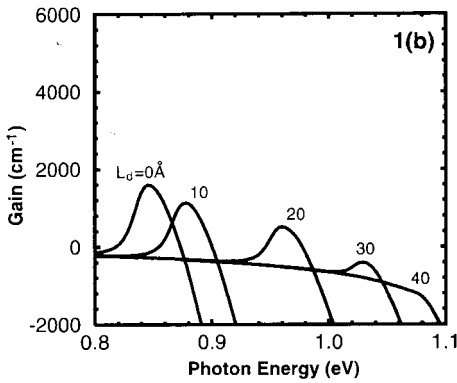
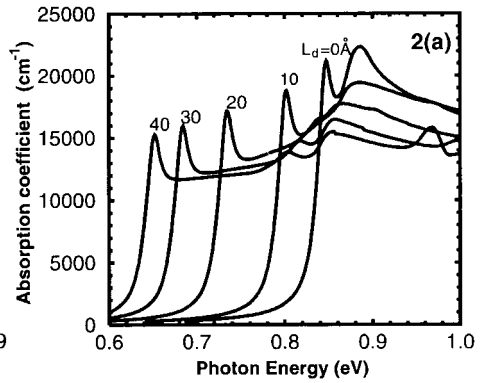
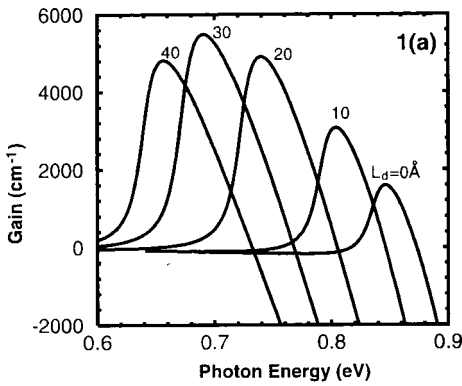


Fig. 1 Optical gain for (a) group-III, (b) group-III & V, and (c) group-V interdiffusion.

Fig. 2 Absorption coefficient for (a) group-III, (b) group-III & V, and (c) group-V interdiffusion.

Table 3 Exciton Binding Energies of interdiffused InGaAs/InP QW (Group V)

Group-V diffusion length (Å)	$L_d=0$	$L_d=10$	$L_d=20$	$L_d=30$	$L_d=40$
HH Binding Energy (meV)	4.84	4.85	4.86	4.87	4.88
LH Binding Energy (meV)	5.92	5.93	5.94	5.95	5.97

In these table, the exciton binding energy decreases (increases) as the diffusion length increases for the only group-III (group-III & V) diffusion. The changes in exciton binding energy for these two diffusion processes are mainly due to the change in the transverse electron and hole effective masses in the well layers. For the two-phase group-V diffusion, the binding energy slight increases as the diffusion length increases.

The absorption coefficients of lattice-matched InGaAs/InP QWs for different diffusion lengths are shown in figure 2. In fig.2(a), we show the absorption of QW with interdiffusion of only group III sublattice. The absorption peak energy also shifts to lower energies as interdiffusion proceeds and the 1s exciton absorption peak decreases with the degree of interdiffusion. The absorption coefficients of wells with interdiffusion of both group-III and group-V sublattices are shown in figure 2(b). This kind of interdiffused QW has the exciton absorption peak shifted to higher energies and increased in the peak height. Figure 2(c) shows the absorption coefficients after the interdiffusion of group V sublattice. It is noticed that the 1s exciton peaks for all the diffused wells have approximately the same energy and the heights of absorption peaks are slightly reduced by interdiffusion.

CONCLUSION

The effects on the optical gain and absorption coefficient of a lattice-matched InGaAs/InP quantum well due to various interdiffusion processes are reported. It is shown that the interdiffusion of group-III sublattice increases the peak gain leading to improved performance in lasers and the interdiffusion of group-III & V sublattices increases the exciton absorption coefficients, which can be used to optimize optical modulators.

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