Characterization of band gap in GaAsSb/GaAs heterojunction and band alignment in GaAsSb/GaAs multiple quantum wells

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Abstract

Photoreflectance (PR) and photoluminescence (PL) spectra are used to investigate the band alignment of GaAsSb/GaAs multiple quantum wells (MQWs). PR and PL spectra are measured for strained and unstrained GaAs_{1-x}Sb_x/GaAs heterojunctions and coherently strained MQWs grown on a GaAs substrate by molecular beam epitaxy. The band gaps of the unstrained GaAs_{1-x}Sb_x obtained from PL agree well with $E_g(x) = 1.43 - 1.9x + 1.2x^2$. For the strained heterojunctions, the strain relaxation factor and the Sb mole fraction determined from PR measurements correspond to the results from X-ray diffraction. In the MQWs, the thickness of the GaAsSb layer is less than its critical thickness so the GaAsSb layer is coherently strained and the band gaps of the GaAs_{1-x}Sb_x layers are estimated under this condition. In this study, the indirect transition from the electron levels in the GaAs layer to the hole levels in the GaAsSb layer is smaller than the band gap of the GaAsSb layer in the MQWs indicating that the band alignment of coherently strained GaAs_{1-x}Sb_x/GaAs MQWs must be type-II.

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Keywords: GaAsSb; MQWs; Strain relaxation; Band alignment; PR; PL

1. Introduction

The application of long wavelength optoelectronic devices has recently become more and more extensively. Many different semiconductor structures such as GaAsSb/GaAs single quantum well (QW) [1,2], GaNAsSb/GaAs QW [3,4], InAs/GaAs quantum dots (QDs) [5], GaAsSb–GaInAs/GaAs bilayer quantum well (BQW) [6,7], GaAsSb/GaAs multiple quantum wells (MQWs) [8], and GaInNAs/GaAs MQWs [9] have been developed. 1.3 μm wavelength laser diodes have attracted special attention due to their minimum losses in optical fiber communication. GaAsSb is a new material in this field and can be used for fiber optics communications, light emitting diodes, photodiodes, etc. For GaAsSb/GaAs quantum wells, a majority of the band offset occurs in the valence band, and the valence-band edge of GaAsSb is higher than that of GaAs. Because of slight conduction-band offset, both weak type-I [10–12] and weak type-II [13–19] band alignments for GaAsSb/GaAs quantum

wells have been reported in the literature. Type-I band alignment describes a conventional system, where electrons and holes are confined in the same layer. For type-II band alignment, electrons and holes confined in different layers causes a spatially indirect transition in the narrow region near the interface. Therefore, the characterization of the band alignment of GaAsSb/GaAs quantum wells is important for device design and theoretical modeling.

In this study, room-temperature photoreflectance (PR) and photoluminescence (PL) spectra were employed to investigate the GaAsSb/GaAs heterojunctions and GaAsSb/GaAs MQWs. The band gap energy of the unstrained GaAsSb and the confined level transitions of the GaAsSb/GaAs MQWs were obtained from the PL spectra and the PR spectra enabled the transition energies of the strained GaAsSb from the conduction-band edge to the heavy-hole and the light-hole band edges, to be obtained. The Sb mole fraction and strain relaxation factor were determined from the valence-band splitting. With the same Sb mole fraction, the PL transition energy of the GaAs_{1-x}Sb_x/GaAs MQWs is smaller than the band gap of the coherently strained GaAs_{1-x}Sb_x. Therefore, the band alignment of coherently strained GaAsSb/GaAs MQWs must be type-II.

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Table 1
Sample structure, Sb mole fraction, and thickness

Sample no.	Structure	Sb mole fraction	Thickness (nm)
A1	GaAsSb/GaAs heterojunction	0.104	GaAsSb 1000 nm/GaAs 300 nm
A2		0.147	
A3		0.223	
A4		0.259	
A5		0.306	
B1	GaAsSb/GaAs heterojunction	0.036	GaAsSb 200 nm/GaAs 300 nm
B2		0.073	
B3		0.134	
B4		0.190	
B5		0.234	
C1	GaAsSb/GaAs MQWs	0.146	Five composite layers, each of GaAsSb 5 nm/GaAs 30 nm
C2		0.223	
C3		0.270	
C4		0.313	
C5		0.340	
C6		0.355	

2. Experiment

Three sets of GaAsSb samples grown on a semi-insulating (100) GaAs substrate by gas-source molecular beam epitaxy (GSMBE) were investigated in this study. The GaAsSb/GaAs heterojunctions with several different Sb compositions were deposited on a 300 nm thick GaAs buffer layer. The thicknesses of the GaAsSb layers are 1000 and 200 nm for sample sets A and B, respectively. In sample set C, the structure of the multiple quantum wells (MQWs) contained a 300 nm thick GaAs buffer layer, five layers of alternating GaAsSb 5 nm/GaAs 30 nm, and a 100 nm thick GaAs cap layer. The sample structures and the Sb mole fraction obtained from X-ray diffraction (XRD) analysis are summarized in Table 1.

For PR measurement, a He–Ne laser served as the pump beam. The probe beam was generated a tungsten lamp and passed through a 1/4 m monochromator. The pump beam was defocused onto the sample with its intensity maintained at $0.10 \mu\text{W}/\text{cm}^2$, therefore the photovoltaic effect induced by the pump beam was very small and negligible. The detection scheme comprised of an InGaAs photodetector and a lock-in amplifier. All measurements were performed at room temperature and at a modulation frequency of 200 Hz. PL was measured at room temperature with the 532 nm line of a solid-state laser as the excitation source. The laser is focused on the sample and chopped for lock-in techniques.

3. Results and discussion

According to Vegard's law, linear interpolation between the lattice constant of GaAs and GaSb is used to obtain the lattice constant of $\text{GaAs}_{1-x}\text{Sb}_x$ [20]. Since the lattice constant of GaSb is greater than that of GaAs, the lattice constant of $\text{GaAs}_{1-x}\text{Sb}_x$ should also be greater than that of GaAs. The $\text{GaAs}_{1-x}\text{Sb}_x$ layer grown on the GaAs substrate receives the compressive strain which causes the energy band edge shift. For the case of the lattice-mismatch strain in a $\text{GaAs}_{1-x}\text{Sb}_x/\text{GaAs}$ heterojunction,

the strains in the epitaxial plane and the growth direction are given separately by [21]:

$$\varepsilon_{xx} = \varepsilon_{yy} = \frac{a_0 - a(x)}{a(x)} = \varepsilon(x) \quad (1)$$

$$\varepsilon_{zz} = -2 \frac{c_{12}}{c_{11}} \varepsilon(x) \quad (2)$$

where a_0 and $a(x)$ are the lattice constants of the GaAs substrate and $\text{GaAs}_{1-x}\text{Sb}_x$ layer, c_{11} and c_{12} are the elastic stiffness constants. The energy shift in the conduction-band edge of the $\text{GaAs}_{1-x}\text{Sb}_x$ is

$$\begin{aligned} \delta E_c(x) &= E_c(x) - E_{c0}(x) = a_c(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) \\ &= 2a_c \left(1 - \frac{c_{12}}{c_{11}} \right) \varepsilon \end{aligned} \quad (3)$$

where $E_c(x)$ and $E_{c0}(x)$ are the conduction-band edge of the strained and unstrained $\text{GaAs}_{1-x}\text{Sb}_x$, and a_c is the hydrostatic deformation potential for the conduction band. Due to the valence-band splitting, the energy shift in the heavy-hole (HH) and light-hole (LH) band edges of the $\text{GaAs}_{1-x}\text{Sb}_x$ are given by

$$\delta E_{HH}(x) = E_{HH}(x) - E_{v0}(x) = -P_\varepsilon(x) - Q_\varepsilon(x) \quad (4)$$

$$\delta E_{LH}(x) = E_{LH}(x) - E_{v0}(x) = -P_\varepsilon(x) - Q_\varepsilon(x) \quad (5)$$

respectively, where $E_{HH}(x)$ and $E_{LH}(x)$ are the heavy-hole and the light-hole band edges of the strained $\text{GaAs}_{1-x}\text{Sb}_x$, and $E_{v0}(x)$ is the valence-band edge of the unstrained $\text{GaAs}_{1-x}\text{Sb}_x$. $P_\varepsilon(x)$ and $Q_\varepsilon(x)$ are defined as

$$P_\varepsilon(x) = -a_v(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) = -2a_v \left(1 - \frac{c_{12}}{c_{11}} \right) \varepsilon \quad (6)$$

$$Q_\varepsilon(x) = -\frac{b}{2}(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) = -b \left(1 + 2 \frac{c_{12}}{c_{11}} \right) \varepsilon \quad (7)$$

where a_v and b are the hydrostatic and shear deformation potential for the valence band. The band gap $E_{g0}(x)$ of the unstrained

GaAs_{1-x}Sb_x is

$$E_{g0}(x) = E_{c0}(x) - E_{v0}(x). \quad (8)$$

The transition energies from the conduction-band edge to the heavy-hole and the light-hole band edge in the strained GaAs_{1-x}Sb_x are

$$\begin{aligned} E_{C-HH}(x) &= E_c(x) - E_{HH}(x) \\ &= [E_{c0}(x) + \delta E_c(x)] - [E_{v0}(x) + \delta E_{HH}(x)] \\ &= E_{g0}(x) + [\delta E_c(x) - \delta E_{HH}(x)] \end{aligned} \quad (9)$$

$$\begin{aligned} E_{C-LH}(x) &= E_c(x) - E_{LH}(x) \\ &= [E_{c0}(x) + \delta E_c(x)] - [E_{v0}(x) + \delta E_{LH}(x)] \\ &= E_{g0}(x) + [\delta E_c(x) - \delta E_{LH}(x)] \end{aligned} \quad (10)$$

respectively. Because the thickness of the GaAs_{1-x}Sb_x layer is much greater than the critical thickness, the PL spectra transition energies for the sample set A are equivalent to the band gaps of unstrained GaAs_{1-x}Sb_x. The band gaps of unstrained GaAs_{1-x}Sb_x do not follow the Vegard's law. In Fig. 1, the PL peak positions versus the Sb mole fractions are fitted well with the room-temperature band gaps of the unstrained bulk GaAs_{1-x}Sb_x [22]:

$$E_{g0}(x) = 1.2x^2 - 1.9x + 1.43 \quad (11)$$

proposed by Nahory et al. (solid line).

Fig. 2 shows the room-temperature PR spectra of the GaAs_{1-x}Sb_x epilayer for the sample set B. The line shape of PR spectra is fitted to

$$\frac{\Delta R}{R} = \text{Re} \left(\sum_{j=1}^p A_j e^{i\theta_j} (E - E_{g,j} + i\Gamma_j)^{-m_j} \right) \quad (12)$$

Fig. 1. The solid line is the band gap energy of the unstrained bulk GaAsSb as a function of the Sb mole fraction at room temperature, as proposed by Nahory et al., and the open circles are the band gaps derived from PL measurement in this study.

Fig. 2. The room-temperature PR spectra of the GaAs_{1-x}Sb_x for the sample set B. The triangle symbols indicate the transition energies from the conduction-band edge to the heavy-hole and the light-hole band edge.

where p represents the number of spectral features, E the photon energy, and A_j , θ_j , $E_{g,j}$, and Γ_j are the amplitude, phase factor, energy gap, and broadening parameter of the j th feature, respectively. The parameter m_j depends on the dimension of the critical point. Here, $m_j = 2.5$ is used, corresponding to a three-dimensional critical point. Because of the lattice-mismatch induced valence-band splitting, two transition energies will be obtained in the PR spectra, and p equals 2. In Fig. 2, the triangular symbols indicate the transition energies from the conduction-band edge to the heavy-hole and the light-hole band edge. The transition energy from the conduction-band edge to the heavy-hole band edge is close to the transition energy from the PL measurement. The transition energies obtained from the theoretical calculation mentioned above do not coincide with the results obtained from the PR spectra. For all samples in the sample set B, the calculated transition energy and the valence-band splitting are greater than those obtained from the PR spectra. This is attributed to a partial relaxation of the strain when the thickness of GaAs_{1-x}Sb_x is greater than the critical thickness. The hypothesized strain relaxation percentage r is defined as

$$r = \left(1 - \frac{\varepsilon'}{\varepsilon} \right) \times 100\% \quad (13)$$

$$\varepsilon' = \frac{a_0 - a'(x)}{a'(x)} = \varepsilon(1 - r) \quad (14)$$

where ε' and ε are real and coherent strain separately, and $0 \leq r \leq 1$. While r equals zero, the real strain is coherent; while r equals 1, the real strain is fully relaxed. Hence, the strain ε in Eqs. (3)–(10) needs to be changed to the real strain ε' , and E_{C-HH} and E_{C-LH} both become a function of the Sb mole fraction (x) and the strain relaxation factor r . Except for the band gap of unstrained GaAs_{1-x}Sb_x, the used parameters of GaAs_{1-x}Sb_x are obtained by linear interpolation between the parameters of GaAs and GaSb listed in Table 2 [14] according to the Vegard's law. The Sb mole fraction and the strain relaxation factor are determined by E_{C-HH} and E_{C-LH} obtained from the PR spectra, and listed in Table 3. The results for the Sb mole fraction approximate to those obtained from the XRD analysis. Reference [23] derives a value for the strain relaxation factor equal

Table 2
The parameters of GaAs and GaSb

Parameter	Symbol (unit)	GaAs	GaSb
Lattice constant	a (Å)	5.6533	6.09593
Energy band gap (300 K)	E_g (eV)	1.43	0.73
Elastic stiffness constant	c_{11} (10^{11} dyn/cm ²)	11.879	8.842
Elastic stiffness constant	c_{12} (10^{11} dyn/cm ²)	5.376	4.026
Hydrostatic deformation potential			
For conduction band	a_c (eV)	−7.17	−6.85
For valence band	a_v (eV)	1.16	0.79
Shear deformation potential			
For valence band	b (eV)	−1.7	−2

to 82% for 172.5 nm thick GaAs_{0.61}Sb_{0.39} using the multibeam optical sensor (MOS) technique. Because the strain relaxation factor decreases with the Sb mole fraction and increases with the thickness, the calculated strain relaxation factor for the sample B5 GaAs_{0.766}Sb_{0.234} with a thickness of 200 nm, is predicted around 82%, and the other samples of the set B show the predicted decrease in strain relaxation factor from 82 to 37% as the Sb mole fraction decreases from 0.234 to 0.051.

Ref. [23] also reported that the critical thickness of the GaAs_{0.61}Sb_{0.39} layer is 16 nm and increases with the decrease of the lattice-mismatch between the epilayer and the substrate. Since the lattice-mismatch between GaAs_{1-x}Sb_x and GaAs decreases with the Sb mole fraction of GaAs_{1-x}Sb_x, the critical thickness of GaAs_{1-x}Sb_x with x smaller than 0.39 is greater than 16 nm. In the sample set C, the Sb mole fractions are all smaller than 0.39 and the thickness of the GaAsSb layer is 5 nm, therefore the GaAsSb layer receives coherent strain. By Eq. (9), the band gap of the GaAs_{1-x}Sb_x with coherent strain can be represented as

$$E_{C-HH}(x) = 1.0956x^2 - 1.4288x + 1.4719 + \frac{0.1639}{x - 3.9114} \quad (15)$$

Fig. 3 displays the room-temperature PL spectra of GaAs_{1-x}Sb_x/GaAs MQWs, i.e. sample set C. The peak positions of the PL spectra and the theoretical calculated band gaps of GaAs_{1-x}Sb_x with the coherent strain are listed in Table 4. With the same Sb fraction, the PL transition energy of GaAs_{1-x}Sb_x/GaAs MQWs is smaller than the band gap of coherently strained GaAs_{1-x}Sb_x. Type-I band alignment describes the conventional system, and the transitions of confined levels in a quantum well are always greater than the band gap, since the

Table 3
For the sample set B, the Sb fractions are obtained from XRD analysis, and the Sb fractions and the strain relaxation factors are determined by E_{C-HH} and E_{C-LH} obtained from PR spectra

Sample	XRD	PR	
	x	x	r (%)
B1	0.036	0.051	37
B2	0.073	0.080	50
B3	0.134	0.143	61
B4	0.190	0.195	77
B5	0.234	0.234	82

Fig. 3. The room-temperature PL spectra of the GaAs_{1-x}Sb_x/GaAs MQWs (sample set C).

Table 4
For the sample set C, the PL transitions of the GaAs_{1-x}Sb_x/GaAs MQWs and the theoretical calculated band gaps of the GaAs_{1-x}Sb_x with coherent strain

Sample	GaAs _{1-x} Sb _x /GaAs MQWs (PL measurement (eV))	Band gap of coherently strained GaAs _{1-x} Sb _x (theoretical calculation (eV))
C1	1.238	1.243
C2	1.134	1.163
C3	1.072	1.121
C4	1.032	1.086
C5	1.014	1.067
C6	1.014	1.057

confined levels of electrons and holes are in the same layer. For the GaAs_{1-x}Sb_x/GaAs MQWs, the band alignment must be type-II, as shown in Fig. 4. The PL transition is due to the recombination, in the narrow region near the interface, of the electrons confined in the GaAs layer with the holes confined in the GaAsSb layer. For the sample C1, the intensity of the PL emission is lower than the others and the PL transition energy is close to the band gap of coherently strained GaAsSb. This is attributed to a smaller number of electrons confined in the GaAs layer due to the smaller conduction-band offset between GaAs_{0.854}Sb_{0.146} and GaAs.

Fig. 4. The schematic diagram of type-II band alignment for coherently strained GaAs_{1-x}Sb_x/GaAs MQWs.

4. Conclusion

This study uses PL to confirm that the equation $E_g(x) = 1.43 - 1.9x + 1.2x^2$ is a good representation of the room-temperature band gap of unstrained GaAs_{1-x}Sb_x as a function of the Sb mole fraction. The strain relaxation factors of the GaAs_{1-x}Sb_x/GaAs heterojunctions with a 200 nm thick GaAs_{1-x}Sb_x layers were determined by valence-band splitting obtained from PR spectra. Moreover, the band alignment of coherently strained GaAs_{1-x}Sb_x/GaAs MQWs must be type-II, since the PL transition energy of the GaAs_{1-x}Sb_x/GaAs MQWs is smaller than the band gap of the coherently strained GaAs_{1-x}Sb_x.

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