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−xSbx/GaAs heterojunctions and coherently strained MQWs grown on a GaAs substrate by molecular beam epitaxy. The band gaps of the unstrained GaAs 1−xSbx 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−xSbx 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−xSbx/GaAs MQWs must be type-II.

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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−xSbx/GaAs MQWs is smaller than the band gap of the coherently strained GaAs 1−xSbx. Therefore, the band alignment of coherently strained GaAsSb/GaAs MQWs must be type-II.
the strains in the epitaxial plane and the growth direction are given separately by [21]:

\[ \varepsilon_{xx} = \varepsilon_{yy} = \frac{a_0 - a(x)}{a(x)} = \varepsilon(x) \]

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

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

\[ \delta E_c(x) = E_c(x) - E_{c0}(x) = a_c(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) \]

\[ = 2a_c \left( 1 - \frac{c_{12}}{c_{11}} \right) \varepsilon \]

where \( E_c(x) \) and \( E_{c0}(x) \) are the conduction-band edge of the strained and unstrained GaAs\(_{1-x}\)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 GaAs\(_{1-x}\)Sb\(_x\) are given by

\[ \delta E_{\text{HH}}(x) = E_{\text{HH}}(x) - E_{\text{HH}0}(x) = -P_v(x) - Q_v(x) \]

\[ \delta E_{\text{LH}}(x) = E_{\text{LH}}(x) - E_{\text{LH}0}(x) = -P_v(x) - Q_v(x) \]

respectively, where \( E_{\text{HH}}(x) \) and \( E_{\text{LH}}(x) \) are the heavy-hole and the light-hole band edges of the strained GaAs\(_{1-x}\)Sb\(_x\), and \( E_{\text{HH}0}(x) \) and \( E_{\text{LH}0}(x) \) are the heavy-hole and light-hole band edges of the unstrained GaAs\(_{1-x}\)Sb\(_x\). \( P_v(x) \) and \( Q_v(x) \) are defined as

\[ P_v(x) = -a_v(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) = -2a_v \left( 1 - \frac{c_{12}}{c_{11}} \right) \varepsilon \]

\[ Q_v(x) = -\frac{b}{2}(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) = -b \left( 1 + 2 \frac{c_{12}}{c_{11}} \right) \varepsilon \]

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
\[ E_{g0}(x) = E_{g0}(0) - E_{g0}(x). \] (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
\[ E_{C-HH}(x) = E_c(x) - E_{HH}(x) \]
\[ = [E_{c0}(x) + \delta E_c(x)] - [E_{g0}(x) + \delta E_{HH}(x)] \]
\[ = E_{g0}(x) + [\delta E_c(x) - \delta E_{HH}(x)] \] (9)
\[ E_{C-LH}(x) = E_c(x) - E_{LH}(x) \]
\[ = [E_{c0}(x) + \delta E_c(x)] - [E_{g0}(x) + \delta E_{LH}(x)] \]
\[ = E_{g0}(x) + [\delta E_c(x) - \delta E_{LH}(x)] \] (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 fraction are fitted well with the room-temperature band gaps of the unstrained bulk GaAs$_{1-x}$Sb$_x$ [22]:
\[ E_{g0}(x) = 1.2x^2 - 1.9x + 1.43 \] (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
\[ \Delta R \over R = \text{Re} \left( \sum_{j=1}^{p} A_j e^{i\theta_j} (E - E_{g,j} + i\Gamma_j)^{-m_j} \right) \] (12)
where \( p \) represents the number of spectral features, \( E \) the photon energy, and \( A_j, \theta_j, E_{g,j}, \) and \( \Gamma_j \) 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
\[ r = \left( 1 - \frac{\varepsilon'}{\varepsilon} \right) \times 100\% \] (13)
\[ \varepsilon' = \left( \frac{a_0 - a'(x)}{a'(x)} \right) = \varepsilon(1 - r) \] (14)
where \( \varepsilon' \) and \( \varepsilon \) 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 \( \varepsilon \) in Eqs. (3)–(10) needs to be changed to the real strain \( \varepsilon' \), 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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol (unit)</th>
<th>GaAs</th>
<th>GaSb</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice constant</td>
<td>(a) (Å)</td>
<td>5.6533</td>
<td>6.09593</td>
</tr>
<tr>
<td>Energy band gap (300 K)</td>
<td>(E_g) (eV)</td>
<td>1.43</td>
<td>0.73</td>
</tr>
<tr>
<td>Elastic stiffness constant</td>
<td>(c_{11}) (10^{11} dyn/cm²)</td>
<td>11.879</td>
<td>8.842</td>
</tr>
<tr>
<td>Elastic stiffness constant</td>
<td>(c_{12}) (10^{11} dyn/cm²)</td>
<td>5.376</td>
<td>4.026</td>
</tr>
</tbody>
</table>

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


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

<table>
<thead>
<tr>
<th>Sample</th>
<th>XRD (x) (%)</th>
<th>PR (x) (%)</th>
<th>(r) (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>B1</td>
<td>0.036</td>
<td>0.051</td>
<td>37</td>
</tr>
<tr>
<td>B2</td>
<td>0.073</td>
<td>0.080</td>
<td>50</td>
</tr>
<tr>
<td>B3</td>
<td>0.134</td>
<td>0.143</td>
<td>61</td>
</tr>
<tr>
<td>B4</td>
<td>0.190</td>
<td>0.195</td>
<td>77</td>
</tr>
<tr>
<td>B5</td>
<td>0.234</td>
<td>0.234</td>
<td>82</td>
</tr>
</tbody>
</table>

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 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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References