Photo-modulation spectroscopy of GaBiAs /GaAs layers grown by MBE

Zahida Batool, Jeff Hosea and Stephen J. Sweeney
Advanced Technology Institute and Department of Physics, University of Surrey,
Guildford, Surrey, GU2 7XH, UK

Tom Tiedje
University of Victoria, Canada

1st International workshop on ‘III-V Bismide Materials for IR and Mid IR Semiconductors’
**What is modulated reflectance?**

- Measure sample’s reflectance $R$ as a function of $\lambda$, while it is being modulated by external periodic perturbation: e.g. electric field (Electro-modulated reflectance - ER).

- Using a chopped pump laser beam gives especially useful **Photo-modulated Reflectance (PR)**: non-destructive, non-contact form of ER.

- Periodically-excited carriers $\rightarrow$ modulate internal $E$-fields $\rightarrow$ modulate complex dielectric fn $\varepsilon_1 + i\varepsilon_2 \rightarrow \Delta\varepsilon_1, \Delta\varepsilon_2 \rightarrow$ differential changes $\Delta R$ in reflectivity $R \rightarrow$ **PR signal** $= \Delta R/ R$

---

**Basic PR mechanism**

![Diagram showing the basic PR mechanism](image)
Sample may be in air, on a turntable, x-y translator, in a cryostat, in electrical contacts, diamond anvil cell etc….

Detector (e.g. simple Si photodiode)

Filter

Lenses

Monochromator

Lamp

Filter

Reference

Chopper

Modulation Source (here, a laser)

ΔR signal in general:
- oscillatory & derivative-like,
- centred on critical-point energy of sample

Computer
GaBiAs/GaAs – sample info

Z-axis is the growth direction

<table>
<thead>
<tr>
<th>sample</th>
<th>Bi%</th>
<th>Thickness of GaBiAS layer (nm)</th>
<th>GaAs Cap (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1835</td>
<td>2.3</td>
<td>40</td>
<td>300</td>
</tr>
<tr>
<td>R1829</td>
<td>4.5</td>
<td>30</td>
<td>uncapped</td>
</tr>
<tr>
<td>R1923</td>
<td>8.5</td>
<td>30</td>
<td>------------</td>
</tr>
<tr>
<td>R1914</td>
<td>10.4</td>
<td>30</td>
<td>------------</td>
</tr>
</tbody>
</table>
Obtaining the band gap transitions from PR
PR Spectra of GaBiAs Layers with 2.3%<Bi<10.4% For Bandgap Transition

514nm/153mW
Ar ion laser
Chopped at 333 Hz

InGaAs Detector

PR/PT line shapes fitted using a sum of two Aspnes third derivative functional forms for HH and LH [2]:

$$\Delta R / R = \text{Re} \left[ Ce^{i\theta} (E - E_g + i\Gamma)^{-n} \right]$$
Strain induced Valence Band splitting (VBS)

- 30-40nm GaBiAs thin layers are under compressive strain, creating VBS.

VBS changes at a rate on the order of 14.7meV/Bi% in good agreement with Franceour et al (15.1meV/Bi%).

Spin orbit splitting transition from PR

Energy vs. PR for GaAs and GaBiAs

\( E_g^{\text{so}} \) GaAs

\( E_g^{\text{so}} \) GaBiAs

\( E_g \)

Conduction Band

Valence Band

Wavevector

\( E_g^{\text{so}} \)

PR

Fitted PR

OSC1 (Eso of GaAs)

OSC2 (Eso of GaBiAs)
Room Temperature

514nm/13.5mW laser Chopped at 333 Hz

Si detector
Reduction of Bandgap and Spin orbit Splitting with increase in Bismuth content

GaBiAs HH/LH and energies from fitting of PR/PT

Strain Tensor Components

In plane strain (along x & y direction) and out of plane strain (z-axis, which axis of growth) are opposite.

\[ \varepsilon_{xx} = \left( a_{GaAs} - a_{GaBiAs} \right) / a_{GaBiAs} \]

Where lattice constant of GaBiAs has been calculated by Vegard’s Law

\[ a_{GaBiAs} = (1 - x)a_{GaAs} + xa_{GaBi} \]
\[ a_{GaBi} = 6.324 \text{ Å} \]

\[ \varepsilon_{zz} = -\left( \frac{2C_{12}}{C_{11}} \right) \varepsilon_{xx} \]

\[ a_{GaAs} = 5.65325 \text{ Å}, \; C_{11} = 12.21 \text{ and } C_{12} = 5.66 \quad \text{of GaAs} \]


Strain Effects on Bandgap

- When \( a_{\text{epi}} > a_{\text{sub}} \), then material is under compressive strain as for GaBiAs.
- Energy levels for the HH, LH and Spin orbit splitting states under strain are [7]

\[
E_{g}^{hh} = (E_{g0} + \delta E_{H}) + \delta E_{S} \\
E_{g}^{lh} = (E_{g0} + \delta E_{H}) + \frac{1}{2} (\Delta_o - \delta E_{S}) - \frac{1}{2} \sqrt{(\Delta_o^2 + 2\Delta_o \delta E_{S} + 9 \delta E_{S}^2)} \\
E_{g}^{so} = (E_{g0} + \delta E_{H}) + \frac{1}{2} (\Delta_o - \delta E_{S}) + \frac{1}{2} \sqrt{(\Delta_o^2 + 2\Delta_o \delta E_{S} + 9 \delta E_{S}^2)}
\]

where

\[
\delta E_{S} = b (\varepsilon_{zz} - \varepsilon_{xx}) \\
\delta E_{H} = (a_c + a_v) (2\varepsilon_{xx} + \varepsilon_{zz}) = a(2\varepsilon_{xx} + \varepsilon_{zz})
\]

\( b \) = shear deformation potential
\( a_c \) = conduction band hydrostatic deformation potential
\( a_v \) = valence band hydrostatic deformation potential
\( a = a_c + a_v \)

By solving these equations and using our experimental results \( E_{g}^{hh} \), \( E_{g}^{lh} \) and \( E_{g}^{so} \) we calculated the shear deformation potential ‘b’ for the GaBiAs as well as its unstrained bandgap \( E_{g0} \) and spin orbit splitting \( \Delta_o \).

Shear Deformation Potential of GaBiAs

The deformation potential ‘–b’ is calculated from the measurements of HH/LH splitting, spin orbit splitting energies and values of compressive strain in material. The rate of increase of magnitude of deformation potential is 163meV/Bi%.
By Using our experimental results of $E_{gh}^s$, $E_{lh}^s$ and $E_{so}^s$ calculated strain and deformation potential ‘b’ of GaBiAs, we have calculated the unstrained bandgap $E_{g0}$ and spin orbit splitting $\Delta_o$. 

GaBiAs Bandgap and SO splitting energy from fitting PR, shown for UNSTRAINED case
Resonance of unstrained Bandgap and Spin Orbit Splitting

GaBiAs Bandgap and SO splitting Energies from the Fitted PR, for the unstrained case

- Bismuth %
  - 0
  - 2
  - 4
  - 6
  - 8
  - 10
  - 12

- Energy (eV)
  - 0.2
  - 0.4
  - 0.6
  - 0.8
  - 1.0
  - 1.2
  - 1.4
  - 1.6

- Ego (this work)
- Alberi et al [4]
- \( \Delta_v \)
- Alberi et al [4]
1. GaBiAs layers on GaAs experience compressive strain which creates a valence band splitting increasing at a rate on the order of 14.7meV/Bi%.

2. Magnitude of the shear deformation potential \( b \) for GaBiAs increases with a rate of \( \sim 163 \text{meV/Bi\%} \)

3. By using experimental \( E_{hh}^g, E_{lh}^g \text{ and } E_{so}^{g} \) we have calculated the unstrained band gap and spin orbit splitting \( \Delta_o \), which become resonant with each other for bismuth fraction 10%<Bi<12%.
Thanks