CHAPTER 4

Band Structures and Properties of Bulk Materials

4.1 Introduction

This chapter is structured to study comprehensively the band structure and properties of bulk materials. As some attention was brought to the issues related with heterostructures in Chapter 1, it is very important to fabricate lattice matched heterostructures. In case the layer being fabricated is not lattice matched to the substrate, the structure may result in dangling bonds (due to electrons which do not participate in bonding) which in turn introduces defects in the system. These defects increase the possibility of non-radiative recombination which is undesirable for the performance of optoelectronic devices. The key factor responsible for defects during heteroepitaxy is the mismatch of thermal expansion coefficients and lattice parameters of two materials which in turn result in development of strain in the structure [1].

Even if the lattice constant of layer being fabricated doesn’t match with the lattice constant of substrate, strained layer epitaxy can be employed to grow defect free structures, provided the thickness of layer being grown is less than the critical thickness. The critical thickness is given by following empirical formula;

\[ d_c \cong \frac{a_s}{2|\epsilon|} \]

where \( \epsilon \) is mismatch parameter and \( a_s \) is lattice constant of substrate. Conclusively, we can say that it is important to choose the lattice matched substrate to fabricate heterostructures. In this section of this chapter, the band structure of InGaAs grown on different substrates like GaAs and InAs is studied. The second material of our interest InGaP is also explored for its band structure when grown on different substrates like GaAs, and GaP.

In Figure 1, band structures of bulk materials are shown. Band structure of InGaAs on substrate GaAs (refer figure 1 a) InGaAs on substrate InAs (refer figure 1 b) InGaP on substrate GaAs (refer figure 1 c) and InGaP on substrate GaP (refer figure 1 d) are plotted. These figures give the
information about the magnitude and type of strain existing in the materials. For example, if the heavy hole lies above the light hole, compressive strain occurs; while in case of tensile strain the light hole lies above the heavy hole. Moreover, the separation between heavy and light holes depends on the magnitude of strain. In order to match the lattice constants of bulk and substrate materials, the selection of alloy compositions or mole fraction of bulk material is very important.

Figure 1. Band Structures of (a) InGaAs/GaAs (b) InGaAs/InAs (c) InGaP/GaAs (d) InGaP/GaP material systems.
4.2 Band Structure of InGaP/GaAs

Figure 2 shows the band structure of InGaP/GaAs for different values of mole fraction ‘x’ of Indium (Refer figure 2 (a) for x = 0.1; 2 (b) for x = 0.3; 2 (c) for x = 0.5; 2 (d) x = 0.8.

![Band structure of InGaP/GaAs](image)

**Figure 2.** Band structures of InGaP/GaAs with different mole fractions (a) x = 0.1 (b) x = 0.3 (c) x = 0.5 (d) x = 0.8
The effect of change in mole fraction of Indium on the energy band gap of InGaP/GaAs has also been summarized in figure 3. The energy band gap is found to decrease with increase in In composition. The inset figure shows the variation in lattice constant as a function of mole fraction. Clearly as the composition of In is increased, lattice constant of the structure also increases which in turn lowers the energy band gap of the structure.

The behavior being depicted in our results is in good agreement with the experimental demonstration given by J. Novak et al. [2] who employed MOVPE method to fabricate In$_x$Ga$_{1-x}$P/GaAs epitaxial layers on GaAs substrate. Further, quite similar behavior has also been reported by Jermy W. Nicklas et al. [3] who have employed HSE06 (Heyd-Scuseria-Ernzerh) hybrid functional to determine the compositional dependence of the band structure of alloy semiconductors. They have reported the band gap of InGaP/GaAs to decrease with the decreasing composition of Ga (or increasing composition of In) which increases the reliability of the graphical picture of the case. The effect of temperature on the band gap of InGaP/GaAs is also studied and it is found that the energy band gap reduces as the temperature is increased as shown in figure. 4

![Figure 3. Band gap of InGaP/GaAs as a function of mole fraction of In.](image)
Figure 4. Effect of temperature on the energy band gap of InGaP/GaAs.

4.3 Band Structure of InGaAs/GaAs

The band structure of InGaAs/GaAs for different values of mole fraction ‘x’ of Indium are plotted in figure 5 (Refer figure 5 (a) for x = 0.1; 5 (b) for x = 0.3; 5 (c) for x = 0.5; 5 (d) x = 0.8. Figure 6 shows the summarized plot of variation in band gap as a function of mole fraction ‘x’ of Indium. The effect of mole fraction on lattice constant of InGaAs/GaAs is also studied and is plotted as the inset graph in figure 6. The lattice constant of the structure is found to increase and the energy band gap of InGaAs/GaAs is found to decrease with increase in the mole fraction of In.

Very Recently, Petr A. Khomyakov et al. [4] carried out the first principles calculations using local density approximation and hybrid functional approach to find the band structure parameters for InGaAs compounds as a function of In composition. The results of dependence of energy band gap on mole fraction of In, being inferred in our discussions above are in good agreement with the theoretical calculations. The variation in the band gap of InGaAs/GaAs as a function of
increasing temperature is also studied and plotted in figure 7. It is found that the energy band gap reduces as the temperature is increased.

Figure 5. Band structures of InGaAs/GaAs with different mole fractions (a) x = 0.1 (b) x = 0.3 (c) x = 0.5 (d) x = 0.8
Sanjib Kabi [5] *et al.* employed DLTS (Deep Level Transient Spectroscopic) technique to measure conduction band offsets for InGaP/GaAs. The estimated values were reported as conduction band offset $\Delta E_c = 0.198$ eV and valence band offset $\Delta E_v = 0.285$ eV. Scanning
Tunneling Microscopy and Spectroscopy have also been employed by Y. Dong et al. [6] to deduce band offsets for InGaP/GaAs interfaces and the reported values of $\Delta E_c$ and $\Delta E_v$ were $0.10 \pm 0.01$ eV and $0.38 \pm 0.01$ eV respectively. Carlo Ghezzi et al. [7] fabricated lattice matched In$_{0.48}$Ga$_{0.52}$P/GaAs heterostructure by molecular beam epitaxy. They studied the effect of growth environmental conditions on the properties of their proposed structure of study. A conduction band offset of 0.119 eV and a valence band offset of 0.356 was reported. Amita Wadehra et al. [8] successfully demonstrated the accuracy of HSE06 (Heyd-Scuseria-Ernzerh) hybrid functional for determining the band offsets of various semiconductor alloy heterostructures. The values being reported for InGaAs/InP were $\Delta E_c = 0.36$ eV valence band offset $\Delta E_v = 0.38$ eV.

In this study, k.p model was employed to calculate the energy band gap of InGaAs on GaAs substrate as a function of mole fraction ‘x’ of In. The results obtained were compared with Hellwege model and Adachi model and are in good agreement with the theoretical calculations, as shown in figure 8. The band gap energy was found to decrease with increasing compositions of In.

![Figure 8. Behavior of InGaAs/GaAs bandgap with mole fraction based on different models](image-url)
References

4. Petr A. Khomyakov, Mathieu Luisier, and Andreas Schenk “Compositional bowing of band energies and their deformation potentials in strained InGaAs ternary alloys: a first-principles study” Integrated Systems Laboratory, Department of Information Technology and Electrical Engineering, ETH Zurich, Gloriastrasse 35, 8092 Zurich, Switzerland (May 2015).