The aim of this chapter is to determine the bulk properties of the materials which have been utilized in the designing of nanoscale-heterostructures. The heterostructures under study are based on III-V binary, ternary and quaternary semiconducting compound such as GaAs, GaSb, InAs, InSb, InN, InP, AlAs, AlGaAs, InGaP, InGaAs, GaAsSb, InGaAlAs, InGaAsP, InGaAsN etc. The band structures of these materials are studied using k.p theory. Moreover, the calculation made for band structures are done near the Γ point, because for calculation of optical response of the optoelectronic devices, the Γ point is of great interest due to emission or absorption of radiations at this point. That’s why most of the semiconductor materials have direct band gaps near this point. For calculation of band structures near the Γ point, k.p method is very suitable as compare to other methods. In figure 1, the Γ point can be seen at the zone center of three dimension Brillouin zone. Besides the central Γ point, the zone boundaries exhibit additional symmetry points. The X point is shown along ±k_x and ±k_y directions, equivalent to ±k_z directions, which are denoted as the <100> direction. The K point lies in the <110> direction and the L point lies in the <111> direction. However, in our work the Γ point is of great interest which lies in Center of the Brillouin zone, as shown in figure 1.

Figure 1. First Brillouin zone of FCC lattice, showing Γ, L, X, K, U, and W points and their directions.
4.1 Band structures of binary compounds

In this section, the band structures of binary compounds are calculated by using k.p theory. In order to ensure about the calculated results, the outcomes are compared with the results available in the literature. The parameters required for band structure calculation are taken from ref. [1].

**Figure 2.** Band structure of GaAs calculated (a) by using k.p method (b) by DFT method using mBJ without spin-orbit interaction [2].

**Figure 3.** Band structure of GaSb calculated (a) by using k.p method (b) by DFT method using mBJ without spin-orbit interaction [2].
In figures 2 to 7, the direct band gap (near the Γ point) of binary semiconductor compounds GaAs, GaSb, InAs, InSb, InP and AlAs are found to be of the order of ~ 1.42, 0.72, 0.36, 0.19, 1.36 and 3.00 eV, respectively. Further, in figures 2 to 7, it can be observed that at wave vector \( k_{||} = 0 \) (near the Γ point), the heavy and light hole subbands of the valence band are overlapped indicating absence of internal strain which occurs due to lattice mismatch.
Figure 6. Band structure of InP calculated (a) by using k.p method (b) by DFT method using mBJ + LDA potential in the X – Γ – L directions of the Brillouin zone [5].

Figure 7. Band structure of AlAs calculated (a) by using k.p method (b) by DFT method using mBJ without spin-orbit interaction [2].
4.2 Band structures of ternary compounds

In this section, the band structures of ternary compounds such as AlGaAs, InGaP, InGaAs, GaAsSb etc. are calculated by using k.p theory.

4.2.1 Band Structure of AlGaAs

![Band Structure of AlGaAs](image)

*Figure 8. Band structure of AlGaAs for mole fraction of ‘Ga’ as (a) 0.2 (b) 0.4 (c) 0.5 and (d) 0.8*

The band structure of the bulk material Al$_{1-x}$Ga$_x$As, pseudomorphically grown on GaAs substrate, has been plotted with different mole fraction of ‘Ga’ in Al$_{1-x}$Ga$_x$As. For mole fraction of 0.2, 0.5, 0.6, and 0.8 of Ga, the band structures have been shown in figure 8 (a), (b), (c) and (d) respectively. In these figures, the conduction band is semi parabolic while the valence sub-
bands are non-parabolic. Moreover, the light and heavy holes valence sub bands are found to coincide at the Γ position which indicates that the bulk material AlGaAs has matched lattice with the GaAs substrate. From all these figures it is clear that the band gap of AlGaAs is decreasing with increasing mole fraction of Ga. The overlapping of light and heavy holes indicates no strain.

4.2.2 Band Structure of InGaP

Figure 9 shows the band structure of InGaP grown on GaAs for different values of mole fraction ‘x’ of Indium. Refer figure 9 (a) for x = 0.1; (b) for x= 0.3; (c) for x= 0.5; (d) x= 0.8.

**Figure 9.** Band structures of InGaP on GaAs with different mole fractions (a) x =0.1 (b) x=0.3 (c) x=0.5 (d) x=0.8
From the figure 9, it is clear that the energy band gap is found to decrease with increase in In composition. The decrease in bandgap due to increase in “In” mole fraction has also been shown in figure 10. The inset picture of figure 10 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 reduce the energy band gap of the structure. Moreover, the existence of tensile strain can be seen (indicating by non-overlapping of light and heavy holes) which results due to lattice mismatch. The results obtained in our work are agreed with the experimental results shown by J. Novak et al. [6] 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. [7] 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.

**Figure 10.** Band gap of InGaP/GaAs as a function of “In” mole fraction.

### 4.2.3 Band Structure of InGaAs

In figure 11, the band structure of InGaAs for different values of mole fraction ‘x’ of Indium are plotted. From figure 11, it can be seen that on increasing the “In” mole faction, the band gap of
InGaAs decrease. This behavior has also been summarized in figure 12. The effect of mole fraction on lattice constant of InGaAs is also studied and plotted in the inset graph of figure 12. The lattice constant of the structure is found to increase and the energy band gap of InGaAs is found to decrease with increase in the “In” mole fraction. Recently, Petr A. Khomyakov et al. [8] have done 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.

Figure 11. Band structures of InGaAs with different mole fractions (a) x =0.1 (b) x=0.3 (c) x=0.5 (d) x=0.8
**4.2.4 Band Structure of GaAsSb**

In recent years, the GaAsSb material system has attracted more attention of researchers belonging to optoelectronic community due its potential for commercial manufacturing of monolithic VCSELs (vertical cavity surface emitting lasers). In the GaAs$_{1-x}$Sb$_x$ material system, the mole fraction of $x=0.36$ has been preferred due to its usage (due to its operation at $\sim 1.3 \, \mu m$) in optical fiber based telecommunication spectrum.

The bulk band structure of the semiconductor compound GaAs$_x$Sb$_{1-x}$, pseudomorphically grown on GaAs substrate, with different mole fraction of ‘As’ in GaAs$_x$Sb$_{1-x}$ has been plotted in figure 13. For mole fraction of 0.3, 0.5, 0.7, and 0.9 of As, the band structures have been shown in figure 13 (a), (b), (c) and (d) respectively. In figure13, for all compositions, the heavy holes are found to lie above the light holes indicating the existence of compressive strain in GaAs$_x$Sb$_{1-x}$ material that comes due to lattice mismatching between GaAs$_x$Sb$_{1-x}$ and GaAs. From this figure, it is also clear that the gap between heavy holes and light holes at the Brillouin zone centre is reduced with increasing the mole fraction of arsenic.
Figure 13. Band structure of GaAsSb/GaAs for mole fraction of ‘As’ as (a) 0.3 (b) 0.5 (c) 0.7 and (d) 0.9

4.3 Band structures of quaternary compounds

In this section, the band structures of quaternary compounds such as InGaAlAs, InGaAsP, etc. are calculated by using k.p theory.

4.3.1 Band structure of InGaAlAs

After studying the band structures of ternary semiconductors such as InGaP, InGaAs, AlGaAs, and GaAsSb, the band structures of quaternary semiconductor InGaAlAs on GaAs substrate has also been studied and shown in figure 14. The energy band degeneracy is missing in this structure as a strain of 3.58 % has been found. This strain may come due to lattice mismatch
between the bulk material grown and the substrate on which the material is grown. Since the strain is compressive the degeneracy has been split largely between the heavy hole and light hole subbands at the zone center. This is because of the difference in the energy Eigen values resulting from different hole masses.

Figure 14. Band structure of InGaAlAs material with x= 0.5 mole fraction of ‘Ga’.

4.3.2 Band structure of InGaAsP

In the figure 15, the band structure (or band dispersion) of bulk material InGaAsP (for Ga = 0.5) grown on InP substrate has been shown. In this figure the light hole sub-band (Green color) is found to lie above the heavy hole sub-band (Red color). This indicates the existence of positive strain (tensile strain) resulting from mismatching between lattice constants of bulk material and substrate on which the bulk material is grown. Moreover, the separation between light hole and heavy hole sub-bands for InGaAsP is found greater than that for InGaAs bulk material. The reason behind this fact is that the strain occurring in the InGaAsP material (~0.038) is greater than that in InGaAs (~0.0022). Here it would be necessary to mention that the split-off holes do not play an important role in the transitions occurring between conduction bands and valence sub-bands because these are found at very below the top of the valence band. Since, some work of the thesis is also related to the optical properties of type-II In_{0.5}Ga_{0.5}As_{0.8}P_{0.2}/GaAs_{0.5}Sb_{0.5}
nano-scale heterostructure; hence the band structure of In$_{0.5}$Ga$_{0.5}$As$_{0.8}$P$_{0.2}$ material system grown on InP substrate is also calculated and plotted in figure 16.

**Figure 15.** Band structure of InGaAsP material system with x = 0.5 mole fraction of ‘Ga’.

**Figure 16.** Band structure of In$_{0.5}$Ga$_{0.5}$As$_{0.8}$P$_{0.2}$ material system grown on InP substrate.
References


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