ABSTRACT

Compound semiconductors which consist of various elements have widely ranging physical properties. It constitutes today's basic building blocks of emitters and receivers in cellular, satellite and fibreglass communication. Semiconductors have attracted much attention in recent years to their great potential for technological importance and have aroused considerably scientific interest. It has therefore become important to understand the electronic structure, elastic properties and the variation of the elastic properties with pressure of binary compound semiconductors. The behavior of a material is predicted by carrying out electronic structure calculations. Elasticity describes the response of a compound to a very small loading which causes reversible deformation. Elastic constant is the fundamental material parameters which characterises the elastic behaviour of a solid. With increase in technology, attempts have also been made to uncover credible alternatives for improving the optoelectronic device performances which has led to the study of III-V alloys. Also the possibility of controlling the physical properties of these alloys in different composition offers immense scope in technological applications studies. Based on these perspectives, the present thesis entitled "**DFT study of some selected Binary Compound Semiconductors: Electronic Structures and Elastic Properties"** have been chosen. This thesis includes a complete study on the structural properties, phase transition, elastic properties and electronic properties of III-V (GaP, GaAs, InP, InAs) and II-VI (ZnS, CdTe and ZnSe) compound semiconductors in both zinc-blende (ZB) and rocksalt (RS) structures under induced pressure in the light of Density Functional Theory (DFT) which is based on electron density rather than the wave function. The effect of InP doped with Ga: $In_xGa_{(1-x)}P$ alloy at different concentration of Ga has also been studied.

The thesis is divided into seven chapters and a detailed layout of these chapters are shown below.

Chapter 1: *Introduction and Review of literature*

This chapter describes the general concepts of compound semiconductors and literature survey on III-V (GaP, GaAs, InP, InAs) and II-VI (ZnS, CdTe and ZnSe) compound semiconductors. It shows the importance of studying the structural properties, phase transition, elastic properties and electronic properties under induced pressure as well as the importance of studying the effect of doping in compound semiconductors.

Chapter 2: *Theoretical methodology*

This chapter describes the theoretical methods used in the present study.

Chapter 3: *Computational tools*

This chapter describes the computational software used in the entire computational calculations of the thesis work.

Chapter 4: *III-V Compound Semiconductors: GaP, GaAs, InP, InAs*

In this chapter, the structural properties of III-V compound semiconductors such as GaP, GaAs, InP and InAs in both zincblende (ZB) and rocksalt (RS) are studied. The structural phase transformation from the ZB to RS structure under induced pressure has also been performed for these compounds and the volume collapse at the transition pressure determined. The elastic constants (C_{11}, C_{12} and C_{44}) of both the ZB and RS phases are found to satisfy the mechanical stability conditions and undergo a linear variation with increase in pressure. The elastic parameters (Zener Anisotropy factor (A), Poisson's ratio (υ), Kleinmann parameter (ζ), B/G ratio, Young's modulus (Y) and Deby's temperature (θ_D)) are also calculated.

The energy band gaps of the ZB and RS structures at zero pressure of GaP, GaAs, InP and InAs are calculated using the LDA, GGA and mBJ-GGA potentials. The implementation of the mBJ-GGA potential in the energy band gap calculation

resolves the underestimation of the band gaps with LDA, GGA and provides better results closer to the experimental value. The corresponding total and partial DOS for the ZB and RS structures at zero pressure are studied within the mBJ-GGA only. The energy band structures as well as the DOS for both ZB and RS structures are studied at different pressures. The energy band gap of ZB phases of GaP, GaAs, InP and InAs are found to be affected by pressure while the energy band gaps of the RS phases are not much affected by pressure.

Chapter 5: *II-VI Compound Semiconductors: ZnS, CdTe, ZnSe*

In this present chapter, we have studied the structural properties of II-VI compound semiconductors, ZnS, CdTe and ZnSe in both ZB and RS structure.

Similar to chapter 4, we have studied the structural phase transition and volume collapse from the zincblende (ZB) to rocksalt (RS) phase of ZnS, CdTe and ZnSe The elastic constants (C_{11}, C_{12} and C_{44}) of both the phases are calculated and found to satisfy the mechanical stability conditions and the corresponding elastic parameters also calculated.

The energy band structures of ZnS, CdTe and ZnSe gaps at zero pressure (in ZB and RS structure) are also calculated using the LDA, GGA and mBJ-GGA methods. The DOS plots for the ZB and RS structures at zero pressure are studied within the mBJ-GGA only and at different pressures. In all the three compounds (ZnS-ZB, CdTe-ZB and ZnSe-ZB) we find that the energy band gap of ZB phases of ZnS, CdTe and ZnSe are affected by pressure while the energy band gaps of the RS phases are not much affected by pressure as in case of the III-V compound semiconductors.

Chapter 6: *Effect of Doping: InP doped with Ga ($In_xGa_{(1-x)}P$)*

In this chapter, the structural phase stability from the zinc-blende (ZB) to rocksalt (RS) structure and electronic structure of $In_{1-x}Ga_{1-x}P$ has been performed to understand the doping effect of Ga in InP compound semiconductor. The lattice parameters of the stable structures of the corresponding doping concentrations are

compared with other available theoretical and experimental results and found to be in good agreement with them. The composition effect on the lattice constant, bulk modulus and the formation energy are studied at different concentration of x (= 0.0, 0.25, 0.5, 0.75, 1) for both B3 and B1 structure. The pressure induce phase transition pressure from B3 to B1 phase in different concentration is found to increase with increase concentration of Ga. For the host binary compounds, the transition pressure is found to be in close agreement with experimental results. The electronic band structure at different concentration of x for both the zinc blende and rock salt structure has been investigated using the total and partial density of states.

Chapter 7: *Overall Conclusion and Outlook*

This chapter presents the overall conclusion of the thesis work (Chapter 4, Chapter 5, Chapter 6) and in future it would be interesting to study the effects of doping in thin films for solar cell studies.

Finally we add an appendix at the end along with the list of publications from the outcome of the results of this dissertation work in referred journal and a list of conference and workshop attended.