The Study of lattice dynamics forms an important part of any course in solid state physics. The vibration of atoms in a crystal not only determine its thermal properties but also govern phenomena like diffuse scattering of X-rays, neutron scattering, spin-lattice relaxation, etc. In order to understand any of these phenomena it is necessary to develop the theory of vibration of atoms, that is the theory of lattice dynamics.

The study of the solid state properties of the semiconducting ternary mixed crystals is of general scientific and technical interest, as these are widely used in I.R. detectors as sensors of thermal radiations and as wide band detectors in the emerging areas of laser radar and laser communication. The properties of mixed crystals of III-V compounds with different band structure may be used in some areas. Due to their wide applications in various fields of science and technology in recent years many studies of mixed systems have also become a subject of considerable theoretical interest.

As the lattice dynamical studies of solids are a pre-requisite for a proper understanding of various properties of solids, the present work has been devoted mainly to the theoretical study of III-V and II-VI Semiconducting mixed crystals of the type $AB_{1-x}C_x$ having zinc-blende structure.

So far no detailed theoretical studies have been made on mixed semiconductors using a reliable model incorporating interatomic interactions in the realistic way. We, therefore, thought it worthwhile to develop a theoretical model for this purpose.

There are three types of compositional vibrations of phonon frequencies. We have studied the two-mode and partly two-mode behaviour of
InP$_{1-x}$As$_x$, Ga$_{1-x}$Al$_x$Sb, GaP$_{1-x}$As$_x$, Cd$_x$Hg$_{1-x}$Te, Mn$_x$Hg$_{1-x}$Te, Cd$_{1-x}$Mn$_x$Te, ZnS$_{1-x}$Se$_x$ and Ga$_{1-x}$In$_x$As, InAs$_{1-x}$Sb$_x$ respectively.

**One-mode behaviour**

In this case, one set of phonon frequency varies with the concentration of the component.

**Two-mode behaviour**

In this case, two sets of phonon frequencies are observed to occur at frequencies close to those of end members.

**Partly two-mode behaviour**

In this case, two sets of phonon frequencies are observed only over certain composition range and one set of phonon frequencies over the remaining composition.

**Chapter 1** of the present thesis describes the development of lattice dynamics of zinc-blende structure. We have briefly mentioned the harmonic approximation and gave formulation of the dynamical matrix. In the harmonic approximation only second order terms in displacement from their equilibrium position in power series expansion of potential energy are retained which involve the displacement. The Green's function technique has been used to obtain the secular determinant for the Crystal structure.

**Chapter 2** describes a brief review of the models previously used by several workers for study of the lattice dynamics of semiconductors. Shortcomings inherent in these models have also been pointed out. These short comings paved the path of the development of a more realistic model.

**Chapter 3** includes description of the dynamical models for mixed semiconductors of the type AB$_{1-x}$C$_x$. An introduction to the model used in the present work is also given in this chapter. Salient features of the Green's
function technique which forms the basis of present studies have been given in
detail in the section 3.5. Concentration dependent Secular determinant as well
as force constants have been obtained and effect of non-randomness have been
discussed in light of two mode behaviour.

Chapter 4 describes the development of present model used by us to
describe various physical, optical and thermal properties of semiconductor of
type II-VI and III-V compounds having zinc-blende structure. The non-Central
rigid ion model (NCRIM) as developed by us is used to explain various
properties of the mixed semiconductors. The potential energy in the framework
of NCRIM comprises two components, one is the non-Coulombic component
and the other is Coulombic component. The non-coulombic considers two-body
interaction. The Coulombic part is calculated using the procedure as developed
by marten. The model involves three bond-stretching in force parameters and
three bond-bending force parameters (corresponding to first and second nearest
neighbour interactions) and one charge parameter due to Coulombic interaction.

These parameters are involved in the elastic constants, phonon
dispersion relations and other lattice dynamic properties of the structure studied
by us. We have evaluated these parameters for end members as well using
experimental data.

Chapter 5 describes the phonon dispersion relations of pure as well mixed
semiconducting compounds. Model parameters in terms of known physical
quantities have also been described in section 5.6. The specific compounds
belonging to II-VI semiconductor group are:

Zns, ZnSe, ZnTe, CdTe, HgTe, MnTe.

And those belonging to III-V group are:

GaP, GaAs, GaSb, InP, InSb, AlSb, InAs.
The mixed semiconductors as studies by us corresponding to II-VI group are:

\[ \text{Cd}_{x}\text{Hg}_{1-x}\text{Te}, \text{Mn}_{x}\text{Hg}_{1-x}\text{Te}, \text{Cd}_{1-x}\text{Mn}_{x}\text{Te}, \text{ZnS}_{1-x}\text{Se}_{x} \]

The mixed semiconductors corresponding to III-V group are:

\[ \text{InP}_{1-x}\text{As}_{x}, \text{Ga}_{1-x}\text{Al}_{x}\text{Sb}, \text{GaP}_{1-x}\text{As}_{x}, \text{Ga}_{1-x}\text{In}_{x}\text{As}, \text{InAs}_{1-x}\text{Sb}_{x} \]

In most of the cases calculated phonon frequencies along [100], [110], and [111] symmetry directions have been found in good agreement with the experimental results for the end members as well as for mixed semiconductors. The two-mode behaviour of mixed semiconductors have also been studies for the composition range \(0 \leq x \leq 1\). Two optical phonon frequencies have been obtained for each value of \(x\). The two-mode behaviour of the mixed system of the type \(AB_{1-x}C_x\) in the three high symmetric directions have also been studied.

**Chapter 6** deals with the thermal properties of II-VI and III-V semiconductor compounds. For this purpose the first Brillouin zone is divided into 1000 miniature cells. The assignment of proper statistical weight reduced these points into 48 non-equivalent points. We have calculated frequencies at all the 48 points. For each point there are six frequencies in the case of end members. The frequency spectrum is divided into intervals of \(\Delta \nu = 0.1\) THz. The density of states \(g(\nu)\) is calculated for each end member as well as their mixed systems. We have used density of states in the calculation of specific heats and corresponding Debye characteristic temperature \(\theta_D\) as a function of temperature. Calculated results have been found in satisfactorily good agreement with available experimental data.

**Chapter 7** deals with the lattice infrared absorption and or Raman spectrum peaks for end members of II-VI and III-V semiconducting compounds. We have calculated critical point phonon frequencies and found that in most of the
cases our calculated results are in close agreement with the experimental data based on Infrared and or Raman measurements. Observed optical peaks for various substances have also been assigned critical point phonon frequencies. The assignments are consistent with Birman's selection rule and support lattice dynamical results. The reliability of the calculated Critical Point phonons for these compounds is checked by Brout's sum rule. Compressibility of various substances as calculated by us compare well with the experimental results.

In this chapter we have also described the importance of mean square displacement in terms of Debye-Waller factor and calculated values of root-mean-square displacement of constituent atoms as a function of temperature. The amplitude of atomic vibration depends upon the temperature. They become large at high temperatures. Eventually a temperature is obtained where the amplitudes are too large to be contained by interatomic forces and there is danger of breaking up of the lattices. **Lindemann states that when the materials attains it melting temperature, the root-mean square amplitude of atomic vibration will be equal to a critical fraction of nearest neighbour distance. The fraction is so called Lindemann's parameter, might be constant and same for all materials, but it has been observed that this fraction in the case of cubic metals and alkali halides is not constant but depends on the crystal structure and the position of the constituent atoms.**

We have calculated the results of II-VI and III-V compound semiconductors and observed that the fraction is nearly constant for II-VI compounds but varies in the case of III-V compound semiconductors.