The study of the non-linear elasticity and elastic anisotropy in crystals, particularly in semiconducting crystals is a subject of great interest. The anharmonicity of crystal lattices can be studied by making use of the higher order elastic constants of crystals. Murnaghan's finite deformation theory and the thermo elastic theory of Thruston and Brugger can be used to study the elasticity in single crystals. Elastic properties link thermodynamically with specific heat, thermal expansion and Grüneisen parameters. Elastic constants of materials are important in technological space applications as the elasticity varies under high pressure and temperature. Theoretical calculations from the thermodynamic and lattice dynamic points are useful in the study of the elastic and thermal properties of crystals.

Lattice dynamics, elastic constants and thermal properties of crystals have great importance in material science also. Elasticity in crystals throws light on the interatomic potentials, equations of state, phonon spectra and lattice specific heat of solids. Second-order elastic constants and their pressure variations provide insight into the nature of the binding forces since they are represented by the derivatives of the free energy of the crystal.

Third-order elastic constants quantify the lowest order anharmonic terms, in the Taylor expansion of the potential energy of a crystal, that influence properties such as thermal expansion. Quantities like lattice thermal
expansion and non-linear elastic constants can be expressed in terms of third-order derivative of the potentials that quantify the coefficients of the cubic term in the expansion of internal energy density and is the leading term in the vibrational anharmonicity of the long wavelength acoustic phonons.

Zinc blende structure has three independent second-order elastic constants and six independent third-order elastic constants. Expressions for the third-order elastic constants are obtained for the interpenetrating cubic system using the Lennard-Jones type of interatomic potential. The second- and third-order elastic constants are used to determine the pressure derivative of the second-order elastic constants and the low temperature limit of the lattice thermal expansion. The elastic stiffness tensor coefficients and their hydrostatic pressure derivatives are used to quantify the vibrational anharmonicity in the long wavelength acoustic-mode phonons to determine the Grüneisen parameters. The Grüneisen parameter is a measure of the lattice thermal expansion of a crystal.

The present study focuses on the second- and third-order elastic constants and the thermal properties of the zinc blende structure II-VI and III-V semiconducting compounds ZnS, ZnSe, ZnTe and GaAs belonging to the \( \bar{4}3m \) point group. The elastic anomalies of these cubic semiconductors have been extensively studied. The advantage of the computational approach is that it can provide a much clearer atomic and electronic picture of the material and
their influence on the structure, properties, synthesis and performances. The present study consists of the following steps.

1. Calculation of interlattice displacements of the crystal.
2. Determination of the second-order elastic constants of the crystal.
3. Determination of the third-order elastic constants of the crystal.
4. Calculation of the pressure derivatives of the second-order elastic constants of the crystal.
5. Determination of the low temperature limit of the lattice thermal expansion of the crystal.

The thesis is divided into seven chapters. Chapter 1 gives a brief review of the II-VI and III-V semiconducting compounds and an introduction to the theory of elasticity and thermal expansion of the crystal. Chapter 2 gives the derivation of the general expressions for the interlattice displacements of the zinc blende structure compounds. The significance of interlattice displacements in these wide gap semiconductors is that it gives the relative displacements of the various lattices that occur when the crystal is strained uniformly. There are eight atoms in the unit cell of these crystals. The interlattice displacements of the various sublattices in the compounds ZnS, ZnSe, ZnTe and GaAs have been determined by taking into account the interactions up to two nearest neighbours of each atom in the unit cell.

Chapter-3 gives the general expressions for the second-order elastic constants of II-VI and III-V compounds ZnS, ZnSe, ZnTe and GaAs. The
values of the second-order elastic constants thus obtained for these compounds are compared with the available experimental data. The second-order elastic constants provide insight into the nature of binding forces between atoms in these crystals since they are represented by the derivatives of the free energy of the crystal. The response of a material to an applied stress is determined by the elastic constants.

In Chapter 4, we obtain the expressions for the third-order elastic constants of the compounds ZnS, ZnSe, ZnTe and GaAs using the method of homogeneous deformation by considering interactions up to two nearest neighbours of each atom in the unit cell. In a non-primitive lattice the macroscopic strain gives rise to interlattice displacements and the method of homogeneous deformation is employed to determine the interlattice displacement of various atoms of the unit cell. It is shown that for the evaluation of the strain energy up to third-order in strains, we need only consider the interlattice displacements up to first order in strains. The complete set of third-order elastic constants of ZnS, ZnSe, ZnTe and GaAs are evaluated and compared with the available experimental values.

Chapter 5 deals with the general expressions for the pressure derivatives of the second-order elastic constants of ZnS, ZnSe, ZnTe and GaAs. The studies on the hydrostatic pressure dependence of the elastic constants of these compounds are necessary for the understanding of the non-linear acoustic properties. The pressure derivatives of the second-order elastic
constants of ZnS, ZnSe, ZnTe and GaAs are determined and compared with available experimental results.

Chapter 6 contains the generalized mode Grüneisen parameters for the interpenetrating FCC compounds ZnS, ZnSe, ZnTe and GaAs. Thermal expansion is a direct consequence of the anharmonicity of the crystal lattice. Here we have evaluated the low temperature limit of thermal expansion of II–VI and III–V semiconducting compounds ZnS, ZnSe, ZnTe and GaAs. In these semiconducting compounds the volume thermal expansion coefficient $\alpha$ at low temperatures is governed by the generalized Grüneisen parameters $\gamma_i(\theta, \phi)$. The low temperature limit of the Grüneisen parameter $\tilde{\gamma}$ is determined using the generalised Grüneisen parameters. The variations in the values of these mode Grüneisen parameters are calculated and plotted as a function of the angle $\theta$, which the direction of propagation makes with the crystal axis in ZnS, ZnSe, ZnTe and GaAs crystals.

Chapter 7 gives the summary and future scope of the work. Most of the work presented in this thesis is in the process of publication. A list of such publications is given below.

1. Elastic constants and pressure derivatives of ZnS.

2. Third-order elastic constants of ZnSe.


3. Higher order elastic constants of ZnTe.


4. Low temperature thermal expansion of wide gap semiconductor ZnSe.


5. *Low temperature Grüneisen gamma* of ZnS.

T.V. Anil, C.S. Menon, and K. Shreekrishna Kumar, *Physica B*. (Communicated)

6. Higher order elastic constants and pressure derivatives of GaAs.


7. Low temperature limit of lattice thermal expansion of ZnTe.