CHAPTER

7

SUMMARY AND CONCLUSION

The interlattice displacements, the second-order elastic constants, third-order elastic constants and the anisotropy in low temperature thermal expansion of the wide gap semiconducting compounds ZnS, ZnSe, ZnTe and GaAs are studied in this thesis. Using the deformation theory, the general expressions for the interlattice displacements of the atoms in the unit cell of ZnS, ZnSe, ZnTe and GaAs have been derived in terms of the strain parameters. While calculating the interlattice displacements, the interactions upto two nearest neighbours have been taken. It is found that the interlattice displacement in these compounds take place in such a way that one type of atoms move with equal amplitude but opposite in direction with respect to the other type of atoms. General expressions for the strain energy of ZnS, ZnSe, ZnTe, and GaAs have been derived using the deformation theory. Comparing the strain energy with the lattice energy density obtained from the continuum model theory, the second- and third-order elastic constants of these compounds are evaluated. The complete sets of second-and third-order elastic
constants of ZnS, ZnSe, ZnTe, and GaAs have been determined and are compared with the available experimental results.

The second-order elastic constants obtained in the present work for these compounds show that the elastic stiffness coefficients of ZnTe are smaller than those of ZnS, ZnSe and GaAs in agreement with the experimental observations. This may be ascribed to the higher bond length of the semiconducting compound ZnTe. The third-order elastic constants which quantify the coefficient of the cubic term in the expansion of strain energy density of ZnS, ZnSe, ZnTe and GaAs are all negative. In all the four compounds, it is found that the absolute value of the longitudinal mode $C_{111}$ is much smaller than that of the shear mode elastic constants like $C_{144}$ and $C_{155}$. This shows the effect of pressure is much greater on shear wave velocity than on the longitudinal wave velocity. The third-order elastic constant forms a sixth-rank tensor, which has in general 729 components. The number of independent constants is reduced by the symmetry considerations. The Cauchy’s relations among the third-order elastic constants for cubic compounds are $C_{112} = C_{155}$ and $C_{123} = C_{456} = C_{144}$. The constants $C_{111}, C_{112}$ and $C_{155}$ are larger in magnitude compared to the constants $C_{123}, C_{144}$ and $C_{456}$. The variation of second-order elastic constants of ZnS, ZnSe, ZnTe and GaAs has also been studied as a function of pressure. The general trends in the change of $C_{11}, C_{12}$ and $C_{44}$ with pressure are similar for all these
semiconductors. \( C_{11} \) and \( C_{12} \) change at nearly the same rate, which is much faster than that for \( C_{44} \).

The low temperature thermal expansion coefficients of the cubic compounds \( \text{ZnS, ZnSe, ZnTe and GaAs} \) are calculated by means of generalised Grüneisen parameters. The low temperature behaviour of the thermal expansion coefficients is governed by the generalised Grüneisen parameters \( \gamma_j (\theta, \phi) \) for acoustic modes propagating in the crystal. The second- and third-order elastic constants have been employed to obtain the generalised Grüneisen parameters. The low temperature limit of the effective Grüneisen parameters \( \bar{\gamma} \) for all the four compounds \( \text{ZnS, ZnSe, ZnTe, and GaAs} \) are evaluated. The variations of mode gamma \( \gamma_j (\theta) \) as functions of \( \theta \) are also studied. The low temperature limit of the volume Grüneisen parameter \( \gamma_L \) obtained in the present work for \( \text{ZnSe and GaAs} \) are compared with available experimental results.

The Grüneisen parameter plays an important role in the studies of contributions of the lattice vibrations to the general properties of semiconductors, since it is a measure of the vibrational anharmonicity. The values of the low temperature thermal expansion \( \bar{\gamma} \) obtained in the present work for these semiconducting cubic crystals \( \text{ZnS, ZnSe and ZnTe} \) show the uniform nature of thermal expansion in these compounds. The low temperature limits of the Grüneisen gammas obtained in the present work for \( \text{II-VI and III-V semiconductors ZnS, ZnSe, ZnTe and GaAs} \) are positive. So
we infer that the volume lattice thermal expansion is positive down to absolute zero in all the four compounds ZnS, ZnSe, ZnTe and GaAs.

The work presented in this thesis can be extended to other similar wide gap semi conducting compounds. The underlying Physics and Chemistry of these semiconducting materials are manifestly quite rich and complex. Since the measured higher order elastic constants of these compounds are not consistent, it requires a remeasurement. A high resolution work on high quality single crystalline samples is needed to determine the higher order elastic constants in these compounds with a greater accuracy. However, considering the implications of the new regimes that arise with the new results reported in this thesis it will help the experimental worker for future measurements.