Preface

Recently, there has been an increased interest in the nonlinear elastic properties of semiconducting crystals. This is connected to the fact that, by altering epitaxial strain on a crystal, the crystal structure can be altered. This structural freedom provides an opportunity for making more efficient and reliable devices by choosing appropriate polytypism. The understanding of the pressure dependence on the elastic constants is decisive in device fabrication and the third order elastic constants provide better understanding of the pressure dependence of the elastic constants. The elastic constants of the semiconducting materials are essential in predicting and understanding the material response, strength, mechanical stability and phase transitions.

In this thesis, the complete sets of non-vanishing second order elastic constants and third order elastic constants of the hexagonal wurtzite phase of cadmium sulphide (CdS), cadmium selenide (CdSe), cadmium telluride (CdTe), aluminium nitride (AlN), gallium nitride (GaN), indium nitride (InN) and silicon carbide (SiC) are obtained using the homogeneous deformation theory. The strain energy is derived using finite strain elasticity theory by considering interactions upto four nearest neighbours of each atom in the unit cell. This is compared with the strain dependent lattice energy density obtained from the continuum model approximation to obtain expressions for the elastic energy density. We also underline the relation of the third order elastic constants to other quantities characterizing anharmonic behaviour of the materials, such as pressure derivatives of the second order elastic constants and the low temperature thermal expansion.
The II-VI, III-V and IV-IV groups of semiconductors are technologically important materials for which the nonlinear effects are particularly significant. The knowledge of the third order elastic constants will improve the design and fabrication of more efficient devices.

The thesis is divided into six chapters:

Chapter 1 gives a brief review of the II-VI, III-V and IV-IV semiconducting crystals. A literature survey is conducted on CdS, CdSe, CdTe, AlN, GaN, InN and SiC with a focus on their structural and mechanical properties.

In Chapter 2, the homogenous deformation theory using the sublattice displacements up to first degree in strain is made use of in calculating the second order elastic constants and third order elastic constants for the hexagonal wurtzite phase of the semiconductors. A procedure to calculate the pressure derivatives of the second order elastic constants and the lattice low temperature thermal expansion from third order elastic constants of the crystals is given.

We determine the second order elastic constants and third order elastic constants of II-VI group semiconductors- CdS, CdSe and CdTe in chapter 3. These elastic constants are used to obtain the first order pressure derivatives and low temperature lattice thermal expansion.

Chapter 4 deals with the calculation of second order elastic constants and third order elastic constants of III-V group semiconductors- AlN, GaN and InN. Using these higher order elastic constants the first order pressure derivatives of the second order elastic constants and low temperature lattice thermal expansion are presented.
Chapter 5 discusses the second order elastic constants and third order elastic constants of IV-IV group semiconductor- SiC. The first order pressure derivatives of second order elastic constants and also the pressure derivatives of elastic moduli of polycrystalline aggregate of SiC are discussed. The low temperature lattice thermal expansion of SiC are calculated using the higher order elastic constants.

In Chapter 6, the results of the present work are summarised. The future scope of this work is also indicated. Most of the work presented in this thesis have either been published or presented in conferences or are in the process of publication.

A list of such publications is given below:

**Publications**


4. **Sindu Jones** and C.S. Menon, *Non-linear elastic coefficients in wurtzite aluminium nitride single crystals under pressure*, (communicated)


12. Sindu Jones and C. S. Menon, Pressure derivatives of the elastic moduli of polycrystalline aggregate of hexagonal wurtzite phase of CdX (X= S, Se) semiconductors from elastic constants of single crystal pressure derivatives, 26th Kerala Science Congress, 28-31 Jan, 2014, Kozhikode.