3.1 Introduction

Second-order elastic constants and their pressure derivatives provide insight into the nature of binding forces between atoms since they are represented by the derivatives of the free energy of the crystal. Further, the response of a material to an applied stress is determined by the elastic constants. The general interest in the large gap semiconductors stimulated numerous theoretical and experimental investigations on the elastic anisotropy of these materials (1-12). Although the second-order elastic constants of these materials received enormous attention, the higher order elastic constants have not been studied comprehensively.

To determine the higher order elastic constants, the complete set of non-vanishing components of second-order elastic constants is necessary. So we have made here an attempt to calculate the complete set of non-vanishing second-order elastic constants of the large gap semiconducting materials ZnS, ZnSe, ZnTe and GaAs.
3.2 Theory

The strain energy expression for large gap semiconductors ZnS, ZnSe, ZnTe and GaAs has been determined using the finite deformation theory (13) and are compared with the strain energy expressions obtained from continuum model (14) to get the expression for the elastic constants in these crystals.

The potential energy per unit cell $\phi$ of crystal can be expanded using Taylor series involving displacement $u$ of the atoms as

$$\phi = \phi_0 + \phi_1 + \phi_2 + \ldots$$

(3.1)

where $\phi_0$ is the static potential energy of the crystal and

$$\phi_1 = \sum_i \phi_i \left( \begin{array}{c} L \\ \mu \end{array} \right) \left( \begin{array}{c} L \\ \mu \end{array} \right)$$

(3.2)

where $u_i \left( \begin{array}{c} L \\ \mu \end{array} \right)$ is the $i$-Cartesian component of $u \left( \begin{array}{c} L \\ \mu \end{array} \right)$.

$u \left( \begin{array}{c} L \\ \mu \end{array} \right)$ is the displacement of the $\mu$th atom in the $L$th unit cell.

$$\phi_2 = \frac{1}{2} \sum_{\mu, \mu'} \phi_{ij} \left( \begin{array}{c} L \\ \mu \end{array} \right) \left( \begin{array}{c} L' \\ \mu' \end{array} \right) u_i \left( \begin{array}{c} L \\ \mu \end{array} \right) u_j \left( \begin{array}{c} L \\ \mu \end{array} \right)$$

(3.3)

where, $\phi_i \left( \begin{array}{c} L \\ \mu \end{array} \right) = \left[ \frac{\partial \phi}{\partial u_i \left( \begin{array}{c} L \\ \mu \end{array} \right)} \right]_{0}$

(3.4)

and

$$\phi_{ij} \left( \begin{array}{c} L \\ \mu \end{array} \right) \left( \begin{array}{c} L' \\ \mu' \end{array} \right) = \left[ \frac{\partial^2 \phi}{\partial u_i \left( \begin{array}{c} L \\ \mu \end{array} \right) \partial u_j \left( \begin{array}{c} L' \\ \mu' \end{array} \right)} \right]_{0}$$

(3.5)
The subscript zero means that the derivatives have to be evaluated in the equilibrium configuration. Here \( \phi \) holds both the translational symmetry of the lattice and the conditions of atomic equilibrium. \( u(L')_{\mu'} \) is the displacement of the \( \mu' \)th atom in the \( L' \)th cell. If we consider interactions under harmonic approximations, it can be noted that \( \phi \) depends only on the square of the vector distance between atoms in the crystal. Under equilibrium condition \( \phi_i \) vanishes and using harmonic approximation, the contribution to the potential energy per unit cell is only from the \( \phi_2 \) term which is the second-order term. Therefore, the change in potential energy when the lattice is homogeneously strained can be written as

\[
\Delta \phi = \phi - \phi_0
\]

\[
= \sum_{i,j} k_2 \left[ \Delta R^2 \left( \begin{array}{c} L \\ \mu \\ \mu' \end{array} \right) \right] 
\]

where

\[
k_2 = \frac{1}{2} \sum_{i,j} \phi_{ij} \left( \begin{array}{c} L \\ \mu \\ \mu' \end{array} \right) 
\]

is the second-order parameter characterising the two body interactions between the pair of atoms \( \left( \begin{array}{c} L \\ \mu \\ \mu' \end{array} \right) \) and \( \left( \begin{array}{c} L' \\ \mu' \end{array} \right) \).

Also, \( \Delta R \left( \begin{array}{c} L \\ \mu \\ \mu' \end{array} \right) = R \left( \begin{array}{c} L \\ \mu \\ \mu' \end{array} \right) \cdot \left( \begin{array}{c} L' \\ \mu' \end{array} \right) \)
where $\mathbf{R}_{L}^{\mu \mu'}$ is the vector distance between the atom $\mu$ in the cell $L$ and atom $\mu'$ in the cell $L'$ in the unstrained state. $\mathbf{R'}_{L}^{\mu \mu'}$ refers to the corresponding vector distance in the strained state. Substituting for $\Delta \mathbf{R}_{L}^{\mu \mu'}$ from equation (2.1) in section (2.2) of chapter 2 in equation (3.6), we get

$$\Delta \phi = 4k_{2} \sum_{L} \sum_{\mu \mu'} \left[ \sum_{ijkl} \mathbf{R}_{i}^{\mu \mu'} \mathbf{R}_{j}^{\mu \mu'} \mathbf{R}_{k}^{\mu \mu'} \mathbf{R}_{l}^{\mu \mu'} \eta_{ij} \eta_{kl} + \sum_{ij} \mathbf{W}_{i}^{\mu \mu'} \mathbf{W}_{j}^{\mu \mu'} \mathbf{R}_{i}^{\mu \mu'} \mathbf{R}_{j}^{\mu \mu'} \right] + 2 \sum_{ijkl} \mathbf{R}_{i}^{\mu \mu'} \mathbf{R}_{j}^{\mu \mu'} \mathbf{R}_{k}^{\mu \mu'} \mathbf{R}_{l}^{\mu \mu'} \mathbf{W}_{i}^{\mu \mu'} \eta_{ij}$$

(3.9)

Since we want terms only up to second-order in Lagrangian strains, we are interested in evaluating their coefficients, we have neglected third and higher powers of $\eta$s here. Here $i$, $j$, $k$ and $l$ are the component indices. $\mathbf{W}(\mu, \mu')$'s are the components of the interlattice displacements of the sublattice $\mu'$ relative to the lattice $\mu$ and $\eta$s are the Lagrangian strains.

Summing up the various components in equation (3.9), we get

$$\Delta \phi = 4k_{2} \sum_{L} \sum_{\mu \mu'} \left[ R_{x}^{2} \mathbf{R}_{x}^{\mu \mu'} \mathbf{R}_{y}^{2} \mathbf{R}_{y}^{\mu \mu'} + R_{y}^{2} \mathbf{R}_{y}^{\mu \mu'} \mathbf{R}_{z}^{2} \mathbf{R}_{z}^{\mu \mu'} + R_{z}^{2} \mathbf{R}_{z}^{\mu \mu'} \mathbf{R}_{z}^{\mu \mu'} \right]$$
\[ + 2 \left[ R_x^2 \left( \mu \mu' \right) R_y^2 \left( \mu \mu' \right) \eta_{xx} \eta_{yy} + R_x^2 \left( \mu \mu' \right) R_z^2 \left( \mu \mu' \right) \eta_{xx} \eta_{zz} \right] \\
+ R_y^2 \left( \mu \mu' \right) R_z^2 \left( \mu \mu' \right) \eta_{yy} \eta_{zz} \right] + 4 \left[ R_y^2 \left( \mu \mu' \right) R_z^2 \left( \mu \mu' \right) \eta_{yz}^2 \right] \\
+ R_z^2 \left( \mu \mu' \right) R_z^2 \left( \mu \mu' \right) \eta_{xz}^2 \right] + R_y^2 \left( \mu \mu' \right) R_y^2 \left( \mu \mu' \right) \eta_{yx}^2 \\
+ R_z^2 \left( \mu \mu' \right) \overline{W}_x \left( \mu, \mu' \right) + R_y^2 \left( \mu \mu' \right) \overline{W}_y \left( \mu, \mu' \right) \\
+ R_z^2 \left( \mu \mu' \right) \overline{W}_z \left( \mu, \mu' \right) \\
+ 2 \left[ R_x \left( \mu \mu' \right) R_y \left( \mu \mu' \right) \overline{W}_x \left( \mu, \mu' \right) \overline{W}_y \left( \mu, \mu' \right) \right] \\
+ R_y \left( \mu \mu' \right) R_z \left( \mu \mu' \right) \overline{W}_x \left( \mu, \mu' \right) \overline{W}_z \left( \mu, \mu' \right) \right] \\
+ R_z \left( \mu \mu' \right) R_z \left( \mu \mu' \right) \overline{W}_x \left( \mu, \mu' \right) \overline{W}_z \left( \mu, \mu' \right) \eta_{xx} \right] \\
+ R_y \left( \mu \mu' \right) R_y \left( \mu \mu' \right) \overline{W}_x \left( \mu, \mu' \right) \overline{W}_z \left( \mu, \mu' \right) \eta_{yy} \right] \]

\[ + 4 \left[ R_x \left( \mu \mu' \right) R_y \left( \mu \mu' \right) R_z \left( \mu \mu' \right) \overline{W}_x \left( \mu, \mu' \right) \overline{W}_y \left( \mu, \mu' \right) \eta_{xy} \right] \\
+ R_y \left( \mu \mu' \right) R_z \left( \mu \mu' \right) \overline{W}_x \left( \mu, \mu' \right) \overline{W}_z \left( \mu, \mu' \right) \eta_{xz} \right] \\
+ R_z \left( \mu \mu' \right) \overline{W}_x \left( \mu, \mu' \right) \eta_{yz} \right] \right) \]

\[(3.10)\]
In wide gap semiconducting compound ZnS, the position co-ordinates of the two nearest neighbours of the atoms in the unit cell are given in Appendix I. The summations in equation (3.10) are carried out for each atom separately. The lattice energy density \( U \) from the continuum model approximation (14) is given by

\[
U = U_0 + \frac{1}{2} \sum_{ijkl} C_{ijkl} \eta_{ij} \eta_{kl} + \ldots
\]

(3.11)

where \( U_0 \) is the lattice energy density in the unstrained state, \( C_{ijkl} \) are the second-order elastic constants defined (15) as

\[
C_{ijkl} = \left[ \frac{\partial^2 U}{\partial \eta_{ij} \partial \eta_{kl}} \right]_{0, S}
\]

(3.12)

Here, the derivatives have to be evaluated under equilibrium conditions and constant entropy \( S \).

Substituting \( W_x, W_y \), and \( W_z \) from equation (2.20) in section 2.2 of chapter 2 in equation (3.10) and by making use of the position co-ordinates of the two nearest neighbours given in the Appendix I, we have

\[
\Delta \phi = k_2 \left[ 16.5 a^4 \eta_{\alpha \alpha}^2 + 32.25 a^4 \eta_{xy}^2 + 17 a^4 \eta_{\alpha \alpha} \eta_{\alpha \alpha} \right]
\]

(3.13)

where \( a \) is the lattice parameter of the crystal.

### 3.3 Second-order Elastic Constants of Zinc Sulphide (ZnS)

Zinc sulphide compound has a structure of zinc blende type, belonging to the face centred cubic \( \bar{4}3m \) point group and the crystal structure is
described by lattice parameter $a = 0.541 \text{ nm}$ (16). The unit cell contains two formula units with Zn tetrahedra occupying the face centred and eight corner sites. ZnS is a II-VI wide gap semiconducting material which received a great deal of attention in recent years in connection with opto-electronic application in the blue spectral region (17,18). Such systems are heterostructures of thin layers, which are stressed and strained due to lattice parameter mismatch. Prediction and analysis of these effects are possible with the help of higher order elastic constants.

Berlincourt et al. (19) have measured the elastic constants of sulphides, selenides and tellurides of zinc and cadmium along with the piezo electric and dielectric constants. For ZnS a bar elongated along [110] with thickness parallel to [001] was used, as well as a square plate perpendicular to [111], allowing a more precise determination of elastic constants. Casali and Christensen (20) have made the theoretical calculations of elastic shear constants and internal strain parameters at the valance band maximum for cubic ZnS and ZnSe under hydrostatic pressure based on density functional theory. The reported values of second-order elastic constants of ZnS by Berlincourt et al. (19) and Casali and Christensen (20) are collected in Table 3.1.

The expressions for second-order elastic constants of ZnS have been obtained by comparing the coefficients of similar powers of the Lagrangian strains in equation (3.13) with those in equation (3.11) for the lattice energy density and using Voigt’s notation, we get
where $V_z$ is the volume of the unit cell of ZnS.

The second-order potential parameter $k_2$ has been obtained from the experimentally measured value of $C_{11}$ from Table 3.1. Using equation (3.14a) and the $k_2$ thus obtained is $k_2 = 0.0429 \times 10^{11}$ newtons/m$^2$. This value of $k_2$ has been used to determine second-order elastic constants of ZnS using equation (3.14). The values of second-order elastic constants for ZnS thus obtained are given in Table 3.1 along with other reported values. Here we have chosen the experimentally measured value of $C_{11}$ by Berlincourt et al. (19) to determine the potential parameter $k_2$.

**Table 3.1** Second-order elastic constants of ZnS (in $10^{11}$ newtons/m$^2$) together with reported values

<table>
<thead>
<tr>
<th>Authors</th>
<th>$C_{11}$</th>
<th>$C_{12}$</th>
<th>$C_{44}$</th>
</tr>
</thead>
<tbody>
<tr>
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<td>1.04</td>
<td>0.54</td>
<td>0.51</td>
</tr>
<tr>
<td>Berlincourt et al. (19)</td>
<td>1.04</td>
<td>0.65</td>
<td>0.46</td>
</tr>
<tr>
<td>Casali and Christensen (20)</td>
<td>1.24</td>
<td>0.62</td>
<td>0.59</td>
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</table>
3.4 Second-order Elastic Constants of Zinc Selenide (ZnSe)

One of the most studied among the II-VI wide gap semiconducting materials is ZnSe which has a zinc blende type structure similar to ZnS. This structure is face centred cubic $\overline{4}3m$ point group with selenium atoms in place of sulphur atoms in ZnS structure. The crystal is described by the lattice parameter $a = 0.567$ nm (18).

Berlincourt et al. (19) has measured the elastic constants of ZnSe along with the piezo electric and dielectric measurements. Lee (21) made the elastic measurements of single crystal ZnSe as a function of temperature over the range 77-300K using the ultrasonic pulse-echo technique. Here, two pieces of single crystal were cut from ingots which consists of many single crystals of different orientation. The crystals were oriented to better than $0.2^{\circ}$ by means of the X-ray Laue back-reflection method, and ground into cubes with plane faces of [100], [1$\overline{1}$0] and [001]. All of the surfaces were polished optically flat and parallel to $10^{-4}$ in./in. The density of samples was measured at 295K by the weight-volume method. The transit time of sound waves was measured by means of the ultrasonic pulse-echo method. Ultrasonic pulses of 1µ sec in duration were introduced into the samples by means of transducers. The longitudinal and transverse waves were generated by X-cut and Y-cut quartz transducers, respectively, operating at their fundamental frequency of 15MHz.

Kuskov et al. (22), Burenkov et al. (23) and Tuchman et al. (24) have measured the values of second-order elastic constants of ZnSe experimentally.
Theoretical calculations of elastic constants of ZnSe by Casali and Christensen (20) based on density functional theory and Sörgel and Scherz (25) based on ab initio calculations. The reported values of the second-order elastic constants of ZnSe are given in Table 3.2.

Comparing the coefficients of similar powers of the Lagrangian strains of the change in potential energy in equation (3.13) with those in equation (3.11) for the lattice energy density, we get the expressions for the second-order elastic constants of ZnSe. The expressions for second-order elastic constants in Voigt’s notation thus obtained are

\[ C_{11} = 24.85 \left( \frac{a_0^5 k_2}{V_z^{3/2}} \right) \]  

\[ C_{12} = 12.8 \left( \frac{a_0^5 k_2}{V_z^{3/2}} \right) \]  

\[ C_{44} = 12.12 \left( \frac{a_0^5 k_2}{V_z^{3/2}} \right) \]  

The potential parameter \( k_2 \) has been obtained from the experimental value of \( C_{11} \) using equation (3.15a) and \( k_2 \) thus obtained is \( k_2 = 0.0346 \times 10^{11} \) newtons/m². The values of second-order elastic constants of ZnSe are obtained using this value of \( k_2 \) in equation (3.15) and are presented in Table 3.2 along with the reported values.
Table 3.2 Second-order elastic constants of ZnSe (in $10^{11}$ newtons/m$^2$) along with the reported values

<table>
<thead>
<tr>
<th>Author</th>
<th>$C_{11}$</th>
<th>$C_{12}$</th>
<th>$C_{44}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Present work</td>
<td>0.86</td>
<td>0.44</td>
<td>0.42</td>
</tr>
<tr>
<td>Lee (21)</td>
<td>0.86</td>
<td>0.51</td>
<td>0.41</td>
</tr>
<tr>
<td>Kuskov et al. (22)</td>
<td>0.94</td>
<td>0.57</td>
<td>0.41</td>
</tr>
<tr>
<td>Tuchman et al. (24)</td>
<td>0.93</td>
<td>0.56</td>
<td>-</td>
</tr>
<tr>
<td>Berlincourt et al. (19)</td>
<td>0.81</td>
<td>0.49</td>
<td>0.44</td>
</tr>
<tr>
<td>Burenkov et al. (23)</td>
<td>0.83</td>
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<td>0.41</td>
</tr>
<tr>
<td>Casali and Christensen (20)</td>
<td>0.96</td>
<td>0.54</td>
<td>0.49</td>
</tr>
<tr>
<td>Sörkel and Scherz (25)</td>
<td>0.98</td>
<td>0.53</td>
<td>0.47</td>
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3.5 Second-order Elastic Constants of Zinc Telluride (ZnTe)

ZnTe belongs to II-VI class of compound and crystallizes in zinc blende form. The zinc blende structure may be viewed as two interpenetrating FCC lattices with Zn atoms are placed on one FCC lattice and Te atoms on the other FCC lattice. The conventional cell is a cube with eight atoms per cell. About each atom there are four equally distant atoms of the opposite kind arranged at the corners of a regular tetrahedron. Zinc blende structure does not have inversion symmetry. Each atom has four nearest neighbours and twelve next nearest neighbours. ZnTe crystal can be described by the lattice parameter $a = 0.61$ nm.
Lee (21) has measured the second-order elastic constants of single crystals of ZnTe as a function of temperature and pressure. The experimental procedure have described in section 3.4. Berlincourt et al. (19) have made the elastic constant measurements of ZnTe along with piezoelectric and dielectric constants. Theoretical contribution of second- and higher order elastic constants is from Sörgel and Scherz (25). The reported values of the second-order elastic constants of ZnTe are given in Table 3.3.

The interlattice displacements $\vec{W}$ for ZnTe obtained from equation (2.23) in section 2.7 of the Chapter 2 are substituted in equation (3.10) and the strain energy per unit volume has been evaluated as in the case of ZnS and ZnSe. Comparing this strain energy density with equation (3.11) for lattice energy density, the expression for the second-order elastic constants of ZnTe, have been evaluated. Using Voigt's notation, these expressions can be written as

$$C_{11} = 25.77 \left( \frac{a^5 k_2}{V_z^{3/2}} \right) \quad (3.16a)$$

$$C_{12} = 13.28 \left( \frac{a^5 k_2}{V_z^{3/2}} \right) \quad (3.16b)$$

$$C_{44} = 12.57 \left( \frac{a^5 k_2}{V_z^{3/2}} \right) \quad (3.16c)$$

We have used the value of Lee (21) to determine the value of $k_2$ from equation (3.16a). The value of $k_2$ has been obtained as $k_2 = 0.0287 \times 10^{11}$ newtons/m² from equation (3.16a). This value of $k_2$ then substituted in equations (3.16), we
have the second-order elastic constants of ZnTe. The second-order elastic constants thus obtained are given in Table 3.3 along with the reported values.

**Table 3.3**  Second-order elastic constants of ZnTe (in $10^{11}$ newtons/m$^2$) together with the reported values

<table>
<thead>
<tr>
<th>Author</th>
<th>$C_{11}$</th>
<th>$C_{12}$</th>
<th>$C_{44}$</th>
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<td>0.38</td>
<td>0.36</td>
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<tr>
<td>Lee (21)</td>
<td>0.74</td>
<td>0.42</td>
<td>0.32</td>
</tr>
<tr>
<td>Berlincourt <em>et al.</em> (19)</td>
<td>0.71</td>
<td>0.41</td>
<td>0.31</td>
</tr>
<tr>
<td>Sörgel and Scherz (25)</td>
<td>0.82</td>
<td>0.42</td>
<td>0.37</td>
</tr>
</tbody>
</table>

3.6  **Second-order Elastic Constants of Gallium Arsenide (GaAs)**

GaAs is the most studied among the III-V semiconducting material. The present objective is to compare the results with somewhat scattered data obtained at room temperature by previous workers. With its zinc blende cubic structure (point group $4\bar{3}m$) GaAs is a piezoelectric material and stiffening of some modes of ultrasonic wave propagation can be expected (26). Its unit cell contains 8 atoms (27) as that of II-VI semiconducting compounds.

The elastic constants at room temperature have been measured by Bateman *et al.*, Garland and Park, Charlso and Mott, Drabble and Brammer, Bobylev and Kravchenko, Meskimin *et al.* and Beilin *et al.* Cottam and Saunders (28) measured the adiabatic elastic constants of GaAs between 2K and 320K using ultrasonic wave velocities by the pulse superposition
technique. Here, to obtain the set of elastic constants in the absence of piezo
electric contributions, choose longitudinal and shear waves propagated along
the [100] direction and the longitudinal wave along the [110]. Transit times were
measured by the pulse superposition technique using a frequency synthesizer
as the repetition-rate oscillator. Measurements were made as a function of
temperature in a standard cryogenic system using gold, 0.02% iron-chromel
and copper-constantan as thermo couples. To generate the shear wave, a dual-
mode transducer was fabricated by the non-perpendicular evaporation scheme.
Garland and Park (29) measured the adiabatic elastic constants of a single
crystal of GaAs over the temperature range 77.4-300K by measuring the
velocities of longitudinal and transverse acoustic waves propagated in the
[110] and [111] directions. Nielsen and Martin (30) made the ab initio
calculations for elastic constants of GaAs. Here, explicit formulae for the
calculations of stress are presented based on the stress theorem and the local
density functional approximation. The reported values of second-order elastic
constants are given in Table 3.4. As in the case of ZnS, ZnSe and ZnTe, by
comparing the coefficients of similar powers of the Lagragian strains of the
change in potential energy in equation (3.13) with those in equation (3.11) for
the lattice energy density, we have the expressions for the second-order elastic
constants of GaAs. The expressions for second-order elastic constants in
Voigt’s notation thus obtained are
The potential parameter has been obtained using the experimental value of \( C_{11} \) given in Table 3.4 using equation (3.17a) and \( k_2 \) thus obtained is \( k_2 = 0.0476 \times 10^{11} \) newtons/m\(^2\). The value of second-order elastic constants of GaAs thus obtained is given in Table 3.4 along with reported values.

**Table 3.4** Second-order elastic constants of GaAs (in \( 10^{11} \) newtons/m\(^2\)) along with the reported values

<table>
<thead>
<tr>
<th>Author</th>
<th>( C_{11} )</th>
<th>( C_{12} )</th>
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</tr>
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<tr>
<td>Cottam and Saunders (28)</td>
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<td>0.59</td>
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<tr>
<td>Garland and Park (29)</td>
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<td>Neilsen and Martin (30)</td>
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<td>0.62</td>
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<tr>
<td>Sörgel and Scherz (25)</td>
<td>1.26</td>
<td>0.55</td>
<td>0.61</td>
</tr>
<tr>
<td>Kitamura * et al. * (34)</td>
<td>1.16</td>
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<td>0.53</td>
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<tr>
<td>San-Guo shen (35)</td>
<td>1.25</td>
<td>0.53</td>
<td>0.51</td>
</tr>
<tr>
<td>Blakemore (37)</td>
<td>1.19</td>
<td>0.54</td>
<td>0.60</td>
</tr>
<tr>
<td>Azuhata * et al. * (36)</td>
<td>1.20</td>
<td>0.55</td>
<td>0.58</td>
</tr>
</tbody>
</table>
3.7 Results and Discussion

Since wide gap semiconducting materials possess cubic symmetry, they exhibit three independent non-vanishing second-order elastic constants. Although many studies have been performed on ZnSe and GaAs, few studies are reported on ZnS and ZnTe. Moreover, the higher order elastic constants of these semiconducting materials are not extensively studied. The results of second-order elastic constants of ZnS obtained in the present work are summarized in Table 3.1. The value of second-order elastic constant $C_{11}$ obtained in the present work is $1.04 \times 10^{11}$ newtons/m$^2$. This is in agreement with the value obtained by Berlincourt et al. (19). The value of $C_{11}$ for ZnS obtained by us differs by 16% from that of Casali and Christensen (20) based on density functional theory. The value of $C_{12}$ reported by Berlincourt et al. (19) for ZnS is $0.65 \times 10^{11}$ newtons/m$^2$. This shows a difference of 17% from our result. They have reported that perfect single crystals in adequate size were not available for effective experimental measurements of elastic constants. The value of $C_{12}$ obtained by us for ZnS differs from that of Casali and Christensen (20) by 13%. The value of shear mode constants obtained by Berlincourt et al. (19) is $0.46 \times 10^{11}$ newtons/m$^2$. This differs from our corresponding $C_{44}$ for ZnS by 11%. Ab initio calculations for $C_{44}$ in ZnS by Casali and Christensen (20) show similar disagreement.

Berlincourt et al.'s (19) experimental value of $C_{11}$ in the case of ZnSe is $0.81 \times 10^{11}$ newtons/m$^2$. Lee (21), Kuskov et al. (22) and Burenkov et al. (23)
have reported the values for $C_{11}$ in ZnSe as $0.86 \times 10^{11}$ newtons/m$^2$, $0.94 \times 10^{11}$ newtons/m$^2$ and $0.83 \times 10^{11}$ newtons/m$^2$ respectively. These values are in agreement with the present result with a slight difference of 0-9%. Tuchman et al. (24) also shows a similar negligible difference for $C_{11}$ values of ZnSe. The present result of ZnSe agrees with some of the theoretical calculations based on density functional theory made by Casali and Christensen (20) and ab initio calculations by Sörgel and Scherz (25). There is a difference of 10% and 12% in $C_{11}$ values of ZnSe.

$C_{12}$ value of ZnSe reported by Berlincourt et al. (19) and Lee (21) agrees well with our results with a difference of 10% and 14% respectively. Although Kuskov et al. (22) and Tuchman et al. (24) disagree with us by 21-23%, in the $C_{12}$ value of ZnSe, Burenkov et al. (23) shows a fairly good agreement. He reported the value for $C_{12}$ in ZnSe as $0.46 \times 10^{11}$ newtons/m$^2$ which differs by 4%. Theoretical calculations from Casali and Christensen (20) and Sörgel and Scherz (25) show a similar disagreement in the case of $C_{12}$ value of ZnSe. Even the experimentally reported values differ considerably among themselves. Experimentally measured value of Berlincourt et al. (19) for $C_{44}$ in ZnSe is $0.44 \times 10^{11}$ newtons/m$^2$. This differs the present value by only 5%. Values reported by the experimental measurements of Lee (21), Kuskov et al. (22) and Burenkov et al. (23) differ the present corresponding results only by 2%. Ab initio calculations of the Casali and Christensen (20) and Sörgel and Scherz (25) obtained the values of $C_{44}$ as $0.49 \times 10^{11}$ newtons/m$^2$ and $0.47 \times 10^{11}$ newtons/m$^2$.
respectively. They differ by a maximum of 14% from the corresponding value obtained by us.

The values of the second-order elastic constants of ZnTe obtained in the present work are summarized in Table 3.3. Berlincourt et al. (19) have made the elastic constant measurements on ZnTe along with piezo electric and dielectric constants. They reported the value of $C_{11}$ as $0.71 \times 10^{11}$ newtons/m$^2$ which is in fair agreement with corresponding value obtained by us. Elastic constant measurement of Lee (21) on single crystal of ZnTe as a function of temperature using ultrasonic pulse-echo technique, gives the value for $C_{11}$ as $0.74 \times 10^{11}$ newtons/m$^2$. This value also is in good accord with present $C_{11}$ result. The corresponding value obtained by Sörgel and Scherz (25) differs by 10%. The $C_{12}$ values of ZnTe of Berlincourt et al. (19) and Lee (21) deviate from our corresponding result by a maximum of 10%. Theoretical work of Sörgel and Scherz (25) in ZnTe also shows a similar disagreement. But the $C_{44}$ value of ZnTe obtained by Berlincourt et al. (19) shows a difference of 16%. The corresponding deviation in the value of $C_{44}$ measured by Lee is 13%. The disagreements among the measurements of elastic constants are attributed to the lack of single crystal in adequate size. Theoretical calculation of the $C_{44}$ value of ZnTe by Sörgel and Scherz (25) is in good accord with our result.

Non-linear elastic properties of GaAs have been a subject of much interest due to its potential applications (31-33). The complete set of second-order elastic constants of GaAs obtained in the present work has been
collected in Table 3.4. Garland and Park (29) have measured the adiabatic elastic constants of gallium arsenide over the temperature range 77-300K by measuring the velocities of longitudinal and transverse acoustic waves propagated in the [110] and [111] directions. He obtained the value for $C_{11}$ as $1.23 \times 10^{11}$ newtons/m² which is in perfect agreement with our result. Ab initio calculations of Nielsen and Martin (30) based on local-density functional approximation and Sörgel and Scherz (25) based on first-principles density functional theory obtained the values of $C_{11}$ for GaAs as $1.23 \times 10^{11}$ newtons/m² and $1.26 \times 10^{11}$ newtons/m² respectively. These differ only by 4% and 6% from our corresponding value respectively. Kitamura et al. (34) has calculated the $C_{11}$ value for GaAs by Hückel Tight-binding (XHTB) method as $1.16 \times 10^{11}$ newtons/m². The corresponding value of San-Guo Shen (35) is $1.25 \times 10^{11}$ N/m² using Bond-Orbital Model (BOM). Theoretical calculations of Azuhata et al. (36) suggested the $C_{11}$ value for GaAs as $1.2 \times 10^{11}$ newtons/m². Meanwhile Blakemore (37) measured the $C_{11}$ component of GaAs as $1.19 \times 10^{11}$ newtons/m². All of the above $C_{11}$ values for GaAs deviate from our corresponding result by 2-6%.

The value obtained by Garland and Park (29) for $C_{12}$ in GaAs is $0.57 \times 10^{11}$ newtons/m² and that of Cottom and Saunders (28) using ultrasonic wave velocity measurement by pulse superposition technique is $0.54 \times 10^{11}$ newtons/m². These values differ by 7% and 13% respectively from the corresponding present value. Kitamura et al. (34) reported the value of $C_{12}$ for GaAs as $0.51 \times 10^{11}$ newtons/m² which shows a difference of 20% from our
corresponding result. Whereas the $C_{12}$ values of San-Guo Shen (35), Blakemore (37) and Azuhata et al. (36) deviate from our corresponding result by 11-15%.

Nielsen and Martin (30) reported the value of $C_{12}$ for GaAs as $0.53 \times 10^{11}$ newtons/m$^2$ using ab initio calculations based on local-density functional approximation. Sörgel and Scherz (25) differ from our corresponding value of $C_{12}$ for GaAs by 11%. The deviation for $C_{44}$ in GaAs obtained by us from those of Garland and Park (29) and Cottom and Saunders (28) is 3% and 2% respectively. The corresponding deviation of Neilsen and Martin (30) and Sörgel and Scherz (25) is 6%. Similar nice agreement can be seen for $C_{44}$ values of GaAs between Kitamura et al. (34), San-Guo Shen (35), Blakemore (37), Azuhata et al. (36) and the present study.

The second-order elastic constants obtained in the present work for ZnS, ZnSe, ZnTe and GaAs show that the elastic stiffness coefficients of ZnTe are smaller than ZnSe, ZnS and GaAs. An accurate remeasurement of elastic constants of ZnS, ZnSe, ZnTe and GaAs is suggested.
References


