Crystal Dynamic Study of Gallium Arsenide (GaAs) using a Theoretical Approach of van der Waals Three-body Force Shell Model (VTSM)

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Authors' Contributions

This work was carried out in collaboration between all authors. KSU designed the study. KKM performed the statistical analysis, wrote the protocol, and wrote the first draft of the manuscript. GKU managed the analyses of the study. KSU managed the literature formatting and manuscript revision. Galley proof has been checked and approved by all the authors.

ABSTRACT

The compound semiconductors of zinc-blende structures (ZBS) are the promising materials for numerous experimental and theoretical investigations. These investigations are the consequences of efforts devoted to understand the interesting crystal properties and interaction mechanism exhibited by these compounds. In this paper we have developed our computed phonon dispersion curve for GaAs along three symmetry directions [q, 0, 0]; [q, q, 0] and [q, q, q] in K-space have been found to be in excellent agreement with the measured inelastic neutron scattering data. We also report Debye temperature variation, two-phonon IR/Raman spectra and anharmonic elastic properties. It is concluded that VTSM is adequately capable of describing the complete crystal dynamic study of zinc-blende structure crystals satisfying well.

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1. INTRODUCTION

Theoretical investigations of the lattice dynamics of III-V semiconductor compounds crystallizing in cubic zinc-blende structure, have been widely studied because of their important semiconducting properties and various applications in the field of non-linear optics, electronics, photovoltaic detectors, LED, solar cells etc. Earlier, Goyal et al. (1978) derived the three elastic constants (C_{11}, C_{12}, C_{44}) for zinc-blende structure. Further, Garg et al. (1978) have investigated the mechanical properties of Zinc-Blende Semiconductor by using Three Body Force Potential (TBFP) and derived the expressions for the third order elastic constants (TOEC) and pressure derivatives of second order elastic constants (SOEC). Later on, these expressions have been used by Singh and coworkers (Singh and Khare, 1981; Singh and Khare, 1982; Singh and Singh, 1982) for calculating the anharmonic properties of Zinc-Blende Semiconducting (ZBS) crystals. However, Sharma and Verma (1980, 1985) have reformulated the expressions derived by Garg et al. (1978) due to errors which were a serious attempt to improve the results. These authors (Sharma and Verma, 1980; 1985) have derived the corrected expressions for Third Order Elastic Constants (TOEC) and pressure derivatives of Second Order Elastic Constants (SOEC) for NaCl, CsCl and ZBS solids. Various workers (Pandey and Upadhyaya, 1978; Upadhyaya et al., 2001, 2002, 2002, 2006; Tiwari et al., 2009, 2010, 2010; Srivastava and Upadhyaya, 2011) used their corrected expressions for calculating the anharmonic elastic properties of only NaCl and CsCl structure crystals. Furthermore, Singh and Singh (1987) implemented these corrected formulations for ZnS, ZnSe and ZnTe, a group of ZBS without inclusion of van der Waals interactions (vWI).

So far, no calculation with corrected formulations have been made for gallium pnictides (GaP, GaAs and GaSb), one of several group III-V compound binary semiconductor crystals. This has motivated the present author to incorporate the effect of van der Waals interaction (VWI) although a weak interaction, quite fundamental in nature to include here in the frame work of both ions polarizable RSM with short range interaction effective up to second neighbor.

From the above description, it may be inferred that the most realistic model proposed purpose can be developed by introducing the effect of VWI in TBI. The present model, known as van der Waals three body force shell model (VTSM), requires 14 parameters computed with the same input (physical properties) for each crystal.

In this paper, we thought it permanent to use the corrected expression mentioned in Singh and Singh (1987) for study of elastic properties, phonon dispersion curve (PDCs) and their pressure dependence for gallium arsenide (GaAs) crystal. The effect of TBI and VWI is quite significant and plays a vital role in the description of the lattice dynamics of gallium pnictides. The proposed investigations have been carried out by adopting a simple method to determine a consistent set of 14 parameters (i.e. four TBI parameters b, , $f(r_0)$, $r_0 f^{'}(r_0)$; two nearest neighbor short-range repulsive interaction parameter parameters A_{12} and B_{12}; four second-nearest-neighbour short- range repulsive interaction parameters A_{11}, B_{11}, A_{22}, B_{22}; distortion polarizabilities of negative and positive ions d_1 and d_2 and shell charges of the negative and positive ions Y_1 and Y_2, respectively) of VTSM. These results have shown reasonably good agreement with their available experimental data (Drable and Brammer, 1966; Waugh and Dolling, 1963; Strauch and Borner, 1990; Mooradian and Bright, 1966; Cochran et al., 1961; Piesebergen, 1963).

The broad outlines about the theoretical framework of present model for calculations have been classified in section 2. The calculated results and their discussions are presented in section 4.

2. THEORETICAL FRAMEWORK OF THE PRESENT MODEL

A detailed description of the Three Body force Shell Model (TSM) has been given by (Singh, 1982). Further we have developed a model which includes the effect of van der Waals interactions (VWI) and three body interactions (TBI) in the framework of RSM and known as van der Waals Three Body Force Shell Model (VTSM). In order to explain the essential theory and method of calculations, a brief idea about the TBP has been given below:

2.1 Three Body Crystal Potential

The present Three Body Force Shell Model for Zinc-Blende Structure (ZBS) semiconductor crystal to describe cohesion, the crystal energy for a particular lattice separation (r) has been expressed as

$$\Phi(r) = \Phi_{LR}(r) + \Phi_{SR}(r) \tag{1}$$

where the first term $_{LR}(r)$ represents the long-range Coulomb and three body interaction (TBI) energies expressed by

$$\Phi_{LR}(r) = -\sum_{\substack{ij \\ i \neq j \neq k}} \frac{Z_i Z_j e^2}{r_{ij}} \left\{ 1 + \sum_k f(r_{ik}) \right\} = -\frac{\ulcorner_M Z^2 e^2}{r} \left\{ 1 + \frac{4}{Z} f(r) \right\} \tag{2}$$

where Z is the ionic charge parameter of ith ion, r_{ij} separation between i^{th} and j^{th} ion, $f(r_{ik})$ is the three body force parameter dependent on nearest-neighbour separation r_{ik} and is a measure of ion size difference (Singh, 1982) and $\ulcorner_M$ is Madelung Constant (=1.63805).

The second term in (1) is short-range energy contributions from overlap repulsion and van der Waals interactions (vdWI) expressed as (Singh and Khare, 1982).

$$\Phi_{SR}(r) = Nb \sum_{i,j=1}^{2} \text{s}_{ij} \exp\left[\frac{r_i + r_j - r_{ij}}{...} \right] - \sum_{ij} \frac{c_{ij}}{r_{ij}^6} - \sum_{ij} \frac{d_{ij}}{r_{ij}^8} \tag{3}$$

where the first term is the Hafemeister and Flygare (HF) potential (Hafemeister and Flygare, 1965) and used by Singh and coworkers (Singh and Singh, 1982; Singh, 1982; Singh and Singh, 1987). The second term and third term represent the energy due to vdW dipole-dipole (d-d) and dipole-quadrupole (d-q) interactions, respectively.

Using the crystal energy expression (1), the equations of motion of two cores and two shells can be written as:

$$\text{Š}^2 \underline{M} \ \underline{U} = (\underline{R} + \underline{Z}_m \ \underline{C}' \ \underline{Z}_m) \ \underline{U} + (\underline{T} + \underline{Z}_m \ \underline{C}' \ \underline{Y}_m) \ \underline{W} \tag{4}$$

$$O = (\underline{T}^T + \underline{Y}_m \ \underline{C}' \ \underline{Z}_m) \ \underline{U} + (\underline{S} + \underline{K} + \underline{Y}_m \ \underline{C}' \ \underline{Y}_m) \ \underline{W} \tag{5}$$

Here $\underline{U}$ and $\underline{W}$ are vectors describing the ionic displacements and deformations, respectively. $\underline{Z}_m$ and $\underline{Y}_m$ are diagonal matrices of modified ionic charges and shell charges, respectively; M is the mass of the core; T and R are repulsive Coulombian matrices,

respectively; *C'* and *Y*$_m$ are long-range interaction matrices, that include Coulombian and TBI respectively; S and K are core-shell and shell-shell repulsive interaction matrices, respectively and T^T is the transpose of matrix T. The elements of matrix $\underline{Z}_m$ consists of the parameter $\underline{Z}_m$ giving the modified ionic charge.

$$Z_m = \pm Z\sqrt{1+(8/Z)f(r_0)} \tag{6}$$

The elimination of $\underline{W}$ from eqns. (4) and (5) leads to the secular determinant:

$$\left| \underline{D}(\vec{q}) - \check{S}^2 \underline{M}\,\underline{I} \right| = 0 \tag{7}$$

for the frequency determination. Here $\underline{D}\,(q)$ is the (6×6) dynamical matrix given by

$$\underline{D}(\vec{q}) = \left(\underline{R}' + \underline{Z}_m\,\underline{C}'\underline{Z}_m\right) - \left(\underline{T} + \underline{Z}_m\,\underline{C}'\underline{Y}_m\right) \times$$
$$\left(\underline{S} + \underline{K} + \underline{Y}_m\,\underline{C}'\underline{Y}_m\right)^{-1}\left(\underline{T}^T + \underline{Y}_m\,\underline{C}'\underline{Z}_m\right) \tag{8}$$

The numbers of adjustable parameters have been largely reduced by considering all the short-range interactions to act only through the shells.

2.2 Second and Third Order Elastic Constants

Proceeding with the use of three body crystal potential given by (1), (Sharma and Verma, 1980, 1985) have derived the expression for the second order elastic constant and used by (Singh and Singh, 1987) for zinc-blende structure crystals. We are reporting them here as their corrected expressions.

The expressions for second order elastic constants (SOEC) are

$$C_{11} = L\left[0.2477Z_m^2 + \frac{1}{3}(A_1 + 2B_1) + \frac{1}{2}(A_2 + B_2) + 5.8243Zaf'(r_0) \right] \tag{9}$$

$$C_{12} = L\left[-2.6458Z_m^2 + \frac{1}{3}(A_1 - 4B_1) + \frac{1}{4}(A_2 - 5B_2) + 5.8243Zaf'(r_0) \right] \tag{10}$$

$$C_{44} = L\left[-0.123Z_m^2 + \frac{1}{3}(A_1 + 2B_1) + \frac{1}{4}(A_2 + 3B_2) - \frac{1}{3}\nabla(-7.539122Z(Z + 8f(r_0)) + A_1 - B_1 \right] \tag{11}$$

and for third order elastic constants (TOEC) they are

$$C_{111} = L\left[\begin{array}{l} 0.5184Z_m^2 + \frac{1}{9}(C_1 - 6B_1 - 3A_1) + \frac{1}{4}(C_2 - B_2 - 3A_2) - 2(B_1 + B_2) - 9.9326Zaf^{'}(r_0) \\ + 2.5220Za^2 f^{''}(r_0) \end{array}\right]$$

(12)

$$C_{112} = L\left[\begin{array}{l} 0.3828Z_m^2 + \frac{1}{9}(C_1 + 3B_1 - 3A_1) + \frac{1}{8}(C_2 + 3B_2 - 3A_2) - 11.642Zaf^{'}(r_0) + \\ 2.5220Za^2 f^{''}(r_0) \end{array}\right]$$

(13)

$$C_{113} = L\left[6.1585Z_m^2 + \frac{1}{9}(C_1 + 3B_1 - 3A_1) - 12.5060Zaf^{'}(r_0) + 2.5220Za^2 f^{''}(r_0)\right]$$ (14)

$$C_{144} = L\left[\begin{array}{l} 6.1585Z_m^2 + \frac{1}{9}(C_1 + 3B_1 - 3A_1) - 4.1681Zaf^{'}(r_0) + 0.8407Za^2 f^{''}(r_0) + \\ \nabla\left\{-3.3507Z_m^2 - \frac{2}{9}C_1 + 13.5486af^{'}(r_0) - 1.681a^2 f^{''}(r_0)\right\} + \\ \nabla^2\left\{-1.5637Z_m^2 + \frac{2}{3}(A_1 - B_1) + \frac{C_1}{9} - 5.3138Zaf^{'}(r_0) + 2.9350Za^2 f^{''}(r_0)\right\} \end{array}\right]$$

(15)

$$C_{166} = L\left[\begin{array}{l} -2.1392Z_m^2 + \frac{1}{9}(C_1 - 6B_1 - 3A_1) + \frac{1}{8}(C_2 - 5B_2 - 3A_2) - (B_1 + B_2) - 4.1681Zaf^{'}(r_0) \\ + 0.8407Za^2 f^{''}(r_0) + \nabla\left\{-8.3768Z_m^2 + \frac{2}{3}(A_1 - B_1) - \frac{2}{9}C_1 + 13.5486af^{'}(r_0) - 1.681a^2 f^{''}(r_0)\right\} + \\ \nabla^2\left\{2.3527Z_m^2 + \frac{C_1}{9} - 5.3138Zaf^{'}(r_0) + 2.9350Za^2 f^{''}(r_0)\right\} \end{array}\right]$$

(16)

$$C_{456} = L\left[\begin{array}{l} 4.897Z_m^2 + \frac{1}{9}(C_1 - 6B_1 - 3A_1) - B_2 + \nabla\left\{-5.0261Z_m^2 - \frac{1}{9}C_1\right\} + \nabla^2\left\{7.0580Z_m^2 + \frac{C_1}{3}\right\} + \\ \nabla^3\left\{-4.8008Z_m^2 + \frac{1}{3}(A_1 - B_1) - \frac{C_1}{9}\right\} \end{array}\right]$$

(17)

where Z_m is the modified ionic charge defined earlier with $L = {e^2}/{4a^4}$ and

$$\nabla = \left[\frac{-7.53912Z(Z + 8f(r_0)) + (A_1 - B_1)}{-3.141Z(Z + 8f(r_0)) + (A_1 + 2B_1) + 21.765Zaf^{'}(r_0)}\right]$$

(18)

The values of A_i, B_i, C_i as defined by Sharma and Verma, (1980; 1985). V (=3.08r_0^2) is the volume of the unit cell.

2.3 Vibrational Properties of Zinc-blende Structure

By solving the secular equation (4) along [$q\,0\,0$] direction and subjecting the short and long-range coupling coefficients to the long-wavelength limit $\vec{q} \to 0$, two distinct optical vibration frequencies are obtained as

$$\left(\sim\check{S}_L{}^2\right)_{q=0} = R_0' + \frac{(Z'e)^2}{\mathsf{v}f_L}\cdot\frac{8f}{3}\left(Z_m{}^2 + 4Zr_0 f'(r_0)\right) \tag{19}$$

$$\left(\sim\check{S}_T{}^2\right)_{q=0} = R_0' - \frac{(Z'e)^2}{\mathsf{v}f_T}\cdot\frac{4f}{3}\,Z_m{}^2 \tag{20}$$

where the abbreviations stand for

$$R_0' = R_0 - e^2\left(\frac{d_1{}^2}{\mathsf{r}_1} + \frac{d_2{}^2}{\mathsf{r}_2}\right); \quad R_0 = \frac{e^2}{V}\left[4\frac{A+2B}{3}\right] ; Z' = Z_m + d_1 - d_2 \tag{21}$$

$$f_L = 1 + \left(\frac{\mathsf{r}_1 + \mathsf{r}_2}{\mathsf{v}}\right)\cdot\frac{8f}{3}\left(Z_m{}^2 + 4Zr_0 f'(r_0)\right) \tag{22}$$

$$f_T = 1 - \left(\frac{\mathsf{r}_1 + \mathsf{r}_2}{\mathsf{v}}\right)\cdot\frac{4f}{3} \tag{23}$$

and $\qquad \mathsf{r} = \mathsf{r}_1 + \mathsf{r}_2$ (24)

2.4 Debye Temperature Variation

The specific heat at constant volume (C_V), at temperature T is expressed as

$$C_V = 3Nk_{\mathbf{B}}\,\frac{\displaystyle\int_0^{\epsilon_m}\left\{\left(h\epsilon/k_B T\right)^2 e^{h\epsilon/k_B T}\right\}G(\epsilon)d\epsilon \Big/ \left(e^{h\epsilon/k_B T} - 1\right)^2}{\displaystyle\int_0^{\epsilon_m}G(\epsilon)d\epsilon} \tag{25}$$

where, ϵ_m is the maximum frequency, N is the Avogadro's a number, h is the Planck's constant and k_B is the Boltzmann's constant. The equation (25) can be written as a suitable form for a computational purpose as

$$C_V = 3Nk_\mathbf{B} \frac{\sum_{\bar{v}} \left\{ \left(h\epsilon / k_B T \right)^2 e^{h\epsilon / k_B T} \right\} G(\epsilon) d\epsilon}{\sum_{\epsilon} G(\epsilon) d\epsilon} \qquad (26)$$

where $E\left(hv / k_B T \right)$ is the Einstein function, defined by

$$E(x) = x^2 \frac{\exp(x)}{\left(\exp(x) - 1 \right)^2} \qquad (27)$$

Also, $\sum_{\epsilon} G(\epsilon) d\epsilon$ = Total number of frequencies considered.

$$= 6000 \text{ for zinc-blende structure.}$$

Hence, equation (21) can be written for zinc-blende structure type crystals, as

$$C_V = \frac{3Nk_B}{6000} \sum_{\epsilon} E(x) G(\epsilon) d\epsilon \qquad (28)$$

The contribution of each interval to the specific heat is obtained by multiplying an Einstein function corresponding to mid-point of each interval (say 0.1 THz) by its statistical weight. The statistical weight of the interval is obtained from the number of frequencies lying in that interval. The contributions of all such intervals when summed up give $\sum_{\epsilon} E(x) G(\epsilon) d\epsilon$. The specific heat C_V is then calculated by expression (28).

3. COMPUTATIONS

There are three basic model parameters ($b, \ldots$ and $f(r_0)$), which have been determined by making use of the expressions for the three second order elastic constants (C_{11}, C_{12}, C_{44}) , derived by (Goyal et al., 1978) and the equilibrium condition, $\left(\dfrac{d\Phi(r)}{dr} \right)_{r=a\frac{\sqrt{3}}{2}=0} = 0$, with inclusion of van der Waals interactions (vdWI). The values of the input data and model parameters have been listed in Table 1. The Values of A_i, B_i, C_i have been calculated from the knowledge of b and ϱ and the values of various order of derivatives of $f(r_0)$ (like $f'(r_0)$, $f''(r_0)$, $f'''(r_0)$) have been obtained by using functional form $f(r_0) = f_0 e^{-r/ \cdots}$ as used by (Singh and Singh, 1987).

The values of vdW coefficients used by us in the present study have been determined using the SKV (Lee, 1970) approach as suggested by (Singh and Singh, 1987). The values of the van der Waals (vdW) coefficients are listed in Table 2. These model parameters and vdW coefficients have been used to compute the rest model parameters $[f(r_0), r_0 f'(r_0), A_{11}, A_{22}, A_{12}, B_{11}, B_{22}, B_{12}, d_1, d_2, Y_1 \text{ and } Y_2]$ of the VTSM further with knowledge of experimental values of the equilibrium interatomic separation *(r₀)*, the vibration

frequencies $\nu_{LO}(X), \nu_{TO}(X), \nu_{LO}(L)$, $\nu_{TO}(L)$, $\nu_{LA}(L)$ and $\nu_{TA}(L)$ and with the values α_1, α_2 $_0$ for gallium pnictides.

The model parameters of VTSM have been used to compute the phonon spectra for zinc-blende structured gallium arsenide (GaAs) for the allowed 48 non-equivalent wave vectors in the first Brillouin zone at Computer Center, Banaras Hindu University, Varanasi. The frequencies along the symmetry directions have been plotted against the wave vector to obtain the phonon dispersion curves (PDCs) from both the models. These curves have been compared with those measured by means of the coherent inelastic neutron scattering technique. Since the neutron scattering experiments provide us only very little data for the symmetry directions, we have studied the combined density of states (CDS) for the complete description of the frequencies for the Brillouin zone.

The complete phonon spectra have been used to calculate the combined density of states (CDS), $N(\nu_j+\nu_{j'})$ corresponding to the sum modes $(\nu_j+\nu_{j'})$, following the procedure of (Smart et al.,1965). A histogram between $N(\nu_j+\nu_{j'})$ and $(\nu_j+\nu_{j'})$ has been plotted and smoothed out to obtain the CDS curves. These curves show well defined peaks which correspond to two-phonon Raman scattering peaks. Since no observed data on two-phonon IR/Raman spectra are available, these CDS peaks have been compared with the assignments calculated by using our present theoretical data and neutron data.

Table 1. Input data and model parameters for GaAs
[C_{ij} and B (in 10^{12} dyne / cm^2), $\in$ (in THz), r_0 (in $10^{>8}$ cm), Γ_i (in 10^{-24} cm^3), b(in 10^{-12} erg), ... (in 10^{-8} cm),]

Input Data		Model Parameters	
Properties	**Values**	**Parameters**	**Values**
C_{11}	11.81[a]	b	0.362
C_{12}	5.23[a]	...	2.69
C_{44}	5.92[a]	$f(r_0)$	-0.248
B	7.62[b]	$r_0 f'(r_0)$	1.6919
r_0	2.47[a]	A_{12}	10.9183
$\in_{LO}(X)$	8.79[c]	B_{12}	-1.1172
$\in_{TO}(X)$	8.13[c]	A_{11}	92.4070
(L)	7.25[c]	B_{11}	-13.56
$\in_{TO}(L)$	7.90[c]	A_{22}	-2.1274
$\in_{LA}(L)$	6.20[c]	B_{22}	-0.9069
$\in_{TA}(L)$	1.9[c]	d_1	0.5124
Γ_1	0.91[d]	d_2	4.3237
Γ_2	7.50[d]	Y_1	-0.2253
$_0$	10.89[e]	Y_2	-3.0632

a- (Garland and Park, 1962); b- (Cotton and Saunders, 1973); c- Waugh and Dolling, 1963);
d- (Shankar et al. 1977); e- (Kunc et al., 1975)

Table 2. Van der Waals Interaction Coefficients for GaAs
(C_{ij} and C in units of 10^{-60} erg cm^6 and d_{ij} and D in units of 10^{-76}erg cm^8)

Parameters	Numerical values
C_{+-}	214
C_{++}	49
C_{--}	1193
d_{+-}	183
d_{++}	16
d_{--}	1062
C	1403
D	882

Furthermore, the division of the Brillouin zone in the present case is somewhat coarse; therefore, the fine structure of the infra-red and Raman shifts may not be reproduced completely. In order to interpret them, the critical point analysis has been used following the method prescribed by (Burstein et al., 1965). Besides above properties, the third order elastic constants (TOEC) and pressure derivatives of second order elastic constants (SOEC) have also been calculated using the VTSM.

For the calculation of Debye Characteristics temperature θ_D at various temperatures, the calculated values of C_V from equation (23) at different temperature T are to be taken and corresponding values (θ_D/T) is determined.

4. RESULTS AND DISCUSSIONS

4.1 Phonon Dispersion Curves

The phonon dispersion frequencies of gallium arsenide (GaAs) have been computed on the basis of present formulation. Inelastic Neutron scattering results for phonon dispersion of this compound have been reported by (Waugh and Dolling, 1963) and later reproduced by (Strauch and Dorner, 1990) with improvement by addition of Raman Scattering Experiments (Sood et al., 1985, 1986). We have computed phonon dispersion frequencies for the allowed 48 non - equivalent wave vectors in the first Brillouin zone by using our model parameters. We present the phonon dispersion curves [PDC] only along the three principal symmetry irections [q, 0, 0], [q, q, 0] and [q, q, q] shown Fig. 1. Our phonon dispersion curves for GaAs agree well with the measured data reported by (Strauch and Dorner, 1990). It is evident from PDCs that our predictions using present model VTSM are better than those by using other models (Kaplan and Sullivan, 1969; Kunc et al., 1970).

4.2 Combined Density of States

The present model is also capable to predict the two phonon Raman/IR spectra. The results of these investigations from combined density states (CDS) approach have been shown in Fig. 2 which shows that the agreement between experimental data and theoretically observed data (Cochran et.al. 1961) and our theoretical peaks is generally good for both two phonon Raman/IR spectra for GaAs. The assignment made by the critical point analysis in the present study has been listed in Table 3. The interpretation of Raman / IR spectra achieved from both CDS approach and critical point analysis is quite satisfactory.
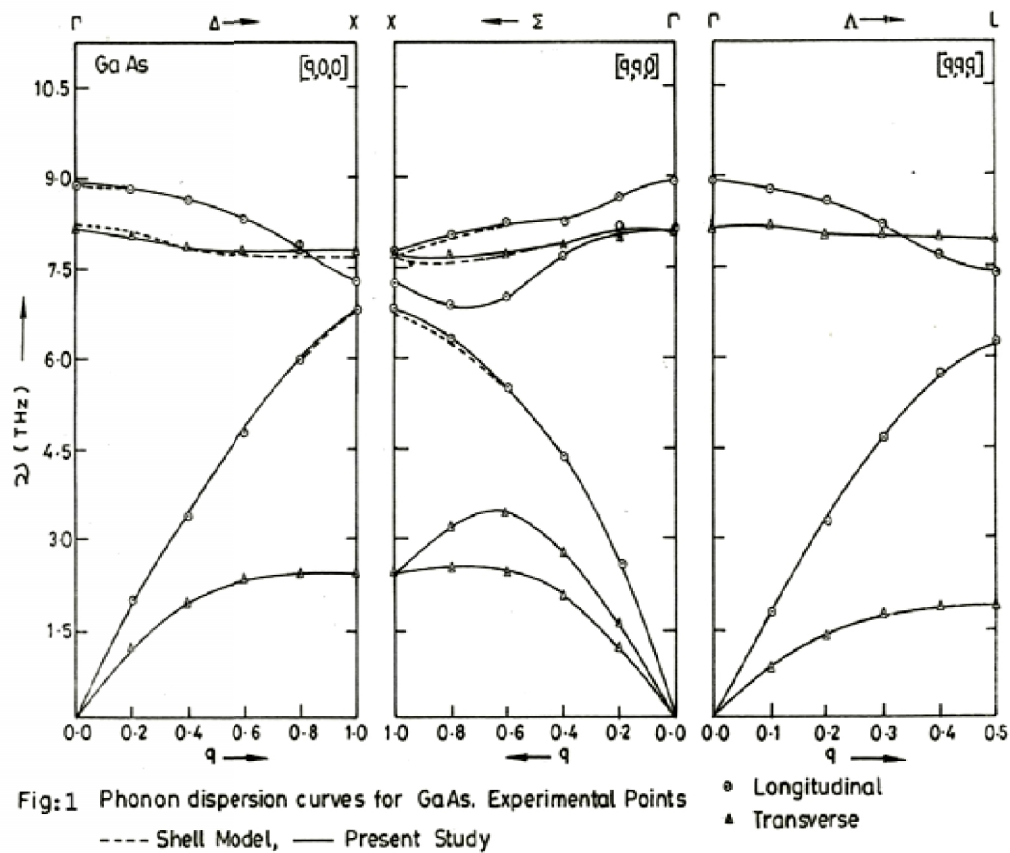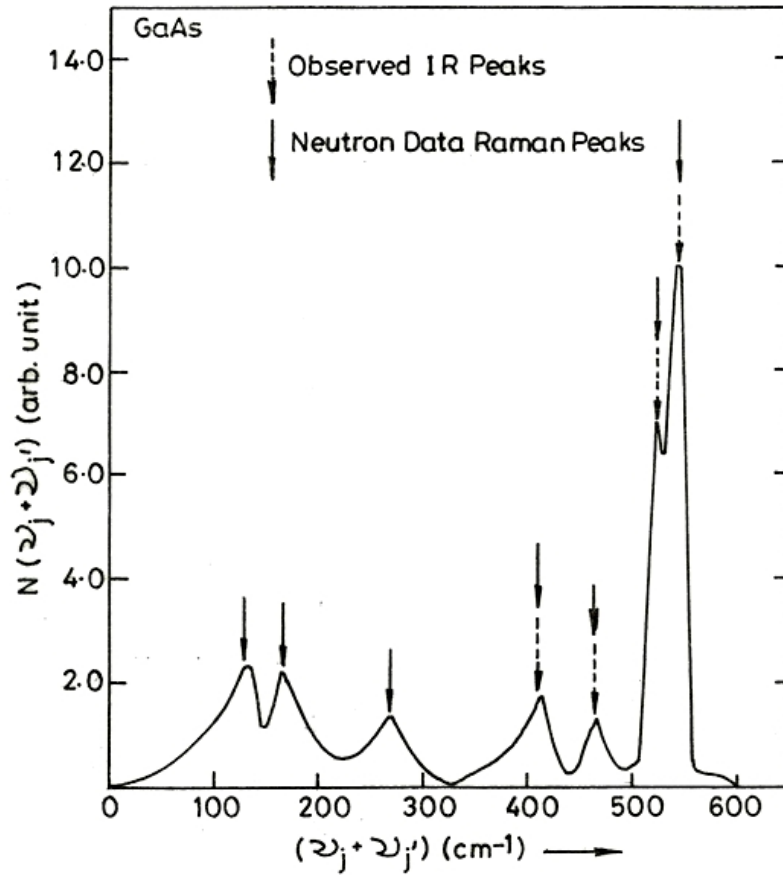
Fig:1 Phonon dispersion curves for GaAs. Experimental Points
---- Shell Model, —— Present Study
Longitudinal
Transverse

Fig. 1. Phonon dispersion curve for GaAs.

Fig. 2. Combined (two phonon) density of states curve for Ga As

Table 3. Assignments for the observed peak positions in Combined Density of States in terms of selected phonon frequencies at , X and L critical points

CDS Peaks (cm^{-1})	Raman Active			Infra-Red Active		
	Neutron Data Peaks (cm^{-1})	Present Study		Observed IR Peaks (cm^{-1})	Present Study	
		Values (cm^{-1})	Assignments		Values (cm^{-1})	Assignments
126	126[f]	126	2TA(L)	…….	…….	…….
164	164[f]	164	2TA(L)	…….	…….	…….
269	269[t]	269	LA(L)+TA(L)	…….	…….	…….
410	412[f]	410	2LA(L)	411[g]	410	2LA(L)
467	469[t]	467	TO(L)+LA(L)	468[g]	468	TO(L)+LA(L)
524	526[f]	524	2TO(L)	524[g]	523	2TO(L)
544	542[f]	544	2TO( )	544[g]	544	2TO( )

f-(Waugh and Dolling, 1963); g- (Cochran et al., 1961)

4.3 Third Order Elastic Constants, Pressure Derivatives of SOECs and Values of Cauchy Discrepancy

It is interesting to note that our results on TOEC and pressure derivatives of SOEC for gallium arsenide (GaAs) are comparable to others are closer to their experimental values. The present model computation of Third order elastic Constants (TOEC) have been reported in Table 4 and compared with the available experimental data (Drable and Brammer, 1966) and other theoretical results (Garg et.al., 1978). Further pressure derivatives of SOEC for GaAs are compared with available experimental data (Miller et. al, 1980) in Table 5. It can also be seen from Table 6 that Cauchy discrepancies are smaller for TOE constants than for SOE constants. A possible explanation for this fact seems to be that many body and/or thermal effects are more pronounced for SOEC than for TOEC.

Table 4. Third Order Elastic Constants (in the unit of 10^{12} dyne/cm^2)

Property	Present Study	Other Theoretical Results	Experimental
C_{111}	-5.851	0.29[h]	-6.75[i]
C_{112}	-4.789	-6.43[h]	-4.02[i]
C_{123}	-1.508	3.29[h]	-0.57[i]
C_{144}	0.214	4.38[h]	0.02[i]
C_{166}	-3.228	-5.71[h]	-3.20[i]
C_{456}	-0.152	3.44[h]	-0.69[i]

h-(Drable and Brammer, 963); i-(Strauch and Dorner, 1990)

Table 5. Values of pressure derivatives of SOEC (in dimensionless) for GaAS

Properties	Values	
	Present Study	Exp.(j)
dK/dP	4.39	4.49[j]
dS/dP	-0.33	0.11[j]
dC_{44}/dP	1.24	1.10[j]

j-(Miller et. al.,1980).

Table 6. Values of Cauchy discrepancy of TOEC (in the unit's 10^{12} dyne cm^{-2}) for GaAs

Properties	Values
$C_{112} > C_{166}$	-1.561
$C_{123} > C_{456}$	-1.356
$C_{144} > C_{456}$	0.366
$C_{123} > C_{144}$	-1.722

4.4 Debye Temperature Variation

Specific Heat C_V values calculated on the basis of present model have presented with better agreement at low temperatures also upto 1^0K which shows predominant with the other zinc-blende semiconductor structure crystals. In the present study the variation of Debye temperatures ($_D$) at different temperatures T have also been calculated and curve has been plotted along with available experimental data (Piesbergen, 1963; Holste, 1972) in Fig. 3. If we start from the lowest temperature first decreases to a minimum, then increases to a

flat maximum and finally decreases slowly. Though, the agreement is better with our model, still, there is slight discrepancy between theoretical and experimental results at higher temperatures.
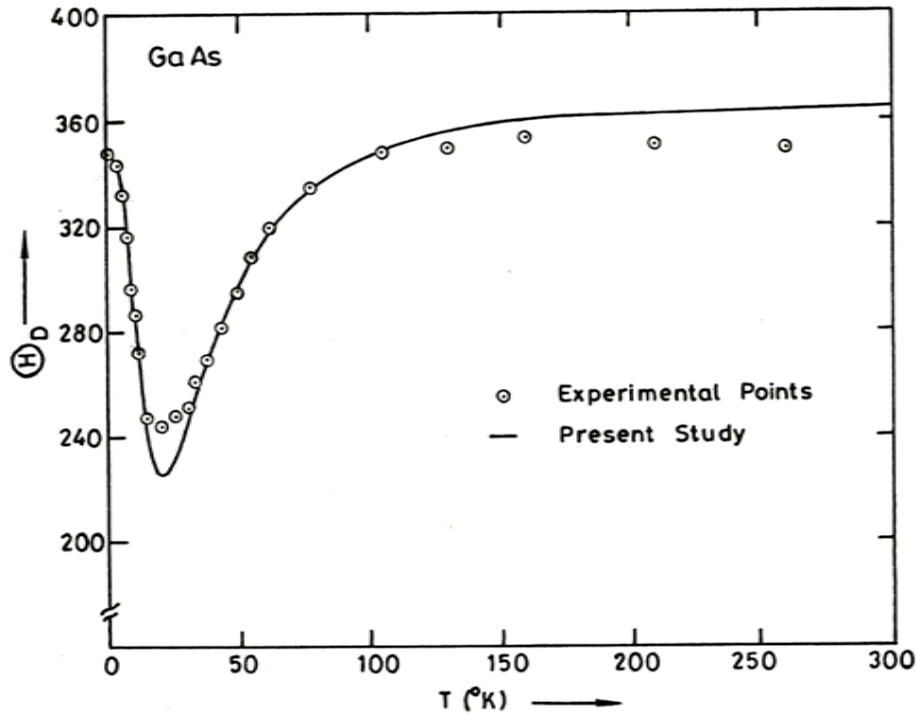

Fig. 3. Debye temperature variation for Ga As

5. CONCLUSION

The computed phonon dispersion curves in Fig. 1 show that inclusion of van der Waals interaction have improved the agreement between experimental data (Waugh and Dolling, 1963; Strauch and Dorner, 1990) and our results. The inclusion of van der Waals interaction (VWI) with (TBI) have influence both longitudinal and transverse optic modes much more than acoustic branches. The agreement between theory and experimental data at X- point is also excellent. Another striking feature of present model is noteworthy from the excellent reproduction of almost all branches hence the prediction of phonon dispersion curves (PDC) for GaAs using (VTSM) may be considered more satisfactory than from other models (Ram And Kushwaha, 1985). The combined density of states (CDS) for GaAs has plotted in Fig. 2 the basic aim of the study of two phonon IR/Raman scattering spectra is to correlate the neutron and optical experimental data of GaAs. We have also investigated the anhormonic properties of GaAs by using VTSM this includes the predictions of third and forth order elastic constants. Here third order elastic constant has been compared with experimental available data (Drable and Brammer, 1966) which shows our result is excellent. We have also plotted Debye temperature curve at temperature (T). It is evident from Fig. 3 our results is good with measured experimental data (Piesbergen, 1963; Holste, 1972) and generally better than of that of valence shell model [VSM].

In this paper, we have systematically reported phonon dispersion curves, combined density of states, Debye temperature and a part of anhormanic property of GaAs. On the basis of overall discussion, it is concluded that the present van der waals three body force shell model (VTSM) is adequately capable of describing the crystal dynamic study of Gallium Arsenide (GaAs).

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COMPETING INTERESTS

Authors have declared that no competing interests exist.

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