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Theoretical Approach of VTSM to Lattice Dynamical Study of Indium Antimonide (InSb)

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Abstract A theoretical study of InSb based on the effect of van der Waal's interactions (VDWI) and three-body interactions (TBI) into the rigid shell model (RSM) of zinc blende structure (ZBS). The van der Waal's three body shell model (VTSM) is performed to analyze the phonon dispersion curves, Debye temperatures variation, combined density of states (CDS) curves, two-phonon Raman and anharmonic elastic properties, where the short range interactions are operative upto the second neighbours. Our results are reasonably good agreement observed between theoretical and experimental data.

Keywords: *phonons, van der Waal's interactions, debye temperature variation, combined density of states curve, phonon dispersion curves, lattice dynamics*

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1. Introduction

Structurally, the most semiconductors consist of a network of covalent bonds leading to an open crystal structure. The general theory of lattice dynamical model [1,2] and in the specific case discussed for phonon dispersion curves for various II- VI and III-V compounds [3,4,5] exhibit tetrahedral coordination under ambient conditions. It gives rise to more dramatic changes in the physical properties of semiconductors than can be attained through temperature variation alone, including band gap closure and metallization. The InSb is a narrow band gap (0.18eV) semiconductor material transition. The molecular lattice dynamical simulation is the choice of the inter-atomic potential, which determines the failure or success of a simulation. In consequence InSb is widely used in infra-red (IR) detectors, lasers and filters etc. The phenomenological models which have been used to calculate the frequencies of ZB crystals classified into two categories (i) rigid-ion model (RIM) [6,7,8] and (ii) rigid-shell model (RSM) [9,10]. The RIM involves the ion rigidity hypothesis; whereas the shell model takes into account the long-range coulomb interaction and also ionic polarizability consideration. The same remarkable theory of Kucher and researcher [11,12] in which the previously developed polarizable atom method [13] is used to calculate the spectrum of diamond type crystals. In constructing a model for a lattice with covalent bonding there is fundamental difficulty related to the introduction of non-central forces [14]. In this usual definition of a non-central interaction [15] the corresponding force parameters are two-centre parameters, while actuality non-central forces cannot be due to rotation of one atom about another, but must be due to a change in the configuration of the atoms or bonds. Hence these force parameters must take into account at least two coordination spheres. The rigid ion model and its various ramifications [16,17,18,19] have been widely used to explain several lattice dynamics properties of perfect and imperfect Z-B type crystals. These model, although economical in force parameters, ignore completely the non-central interaction in the lattice. The valance force field model (VFFM) as used by Price et al. [20] incorporates bond bending, bond-stretching and point coulombic interactions. Later on the original 14 parameter VFFM was modified on the lines of shell model by Vegelatos et al. [5] and Feldkamp et al. [21]. In addition to lattice dynamics by Garg et al. [22], have investigated the mechanical properties of zinc-blende semiconductor by using three body force shell model [TSM] and derive the expressions for the third order elastic constants (TOEC) and pressure derivatives of second order elastic constants (SOEC) on the way of Singh and Verma [23,24]. Analysis of these models RIM [6,7,8]; RSM [9,10]; VFFM [20]; TSM [22,23,24]; BCM [25]; DDM [26] and ECM [27] reveal that the crystal dynamics study of zinc-blende crystals is still not well understood. The present model, known as van der Waals three body force shell model (VTSM), has 14 parameter computed for each crystal with the same input data (physical properties) and VWI has been added to short-range repulsive interactions operative up to second nieghbour. So, it is obvious that along with the TBI, VWI must be taken into consideration in any discussion of lattice dynamics of these crystals. This new

model, VTSM, co-operate VWI along with long range coulomb interactions, TBI and short range second neighbor interactions in the framework of RSM. The effect of TBI and VWI is quite significant and plays a very important role in the description of the lattice dynamics of Indium pnictides (InP, InSb, InAs).

In this communication, we have mainly discussed a theoretical approach of lattice dynamical study of InSb. The experimental data of InSb for phonon dispersion curves [20], harmonic and anharmonic elastic constants [28], Debye temperature variation [16,29,30,31,32], two phonon IR spectra [33,34] are available. The second order IR spectra of InSb, provides additional information of phonon mode frequencies at critical points near the edge of the first Brillion zone. The formalism of our model VTSM has been given by Pandey et al. [35] and also from Dubey et al [36,37,38].

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, ρ, $f(r_0)$, $r_0f''(r_0)$; 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. The broad outlines about the theoretical framework of present model for calculations have been classified in section 2.

2. Method of Calculation

The values of the input data Price et al. [20], Banerjee and Varshni [16], Slutsky and Garland [39], Kunc et al. [40], Hass and Henvis [41] and calculated VTSM model parameters have been shown in Table 1. The values of A_i, B_i, C_i calculated from the knowledge of b, ρ; the values of various order of derivatives of $f(r_0)$ and van der Waal's coupling coefficients. The values of VDW coefficients used by us in the present study have been determined using SKV method [42] as suggested by Singh and Singh [43] and reported by Sharma and Verma [44]. Thus our model parameters are [b, ρ, $f(r_0)$, $r_0f'(r_0)$, A_{12}, A_{11}, A_{22}, B_{12}, B_{11}, B_{22}, d_1, d_2, Y_1 and Y_2]. The values of the VDW coefficients are shown in Table 2. Our model parameters of VTSM used to compute the phonon spectra of InSb for allowed 48 non-equivalent wave vectors in the first Brillouin zone. The frequencies along the high symmetry directions [q00], [qq0] and [qqq] were plotted against the wave vector to obtain the phonon dispersion curves (PDCs). These curves were compared with measured by coherent inelastic neutron scattering technique [45] especially TA modes are very much different not only from ours but from BCM calculations of Rajput and Browne [45] alongwith in Figure 1. Since the neutron scattering experiments provide us very few data for the symmetry directions, we have also computed CDS and the Debye temperature variation for the complete description of the frequencies for the Brillouin zone.

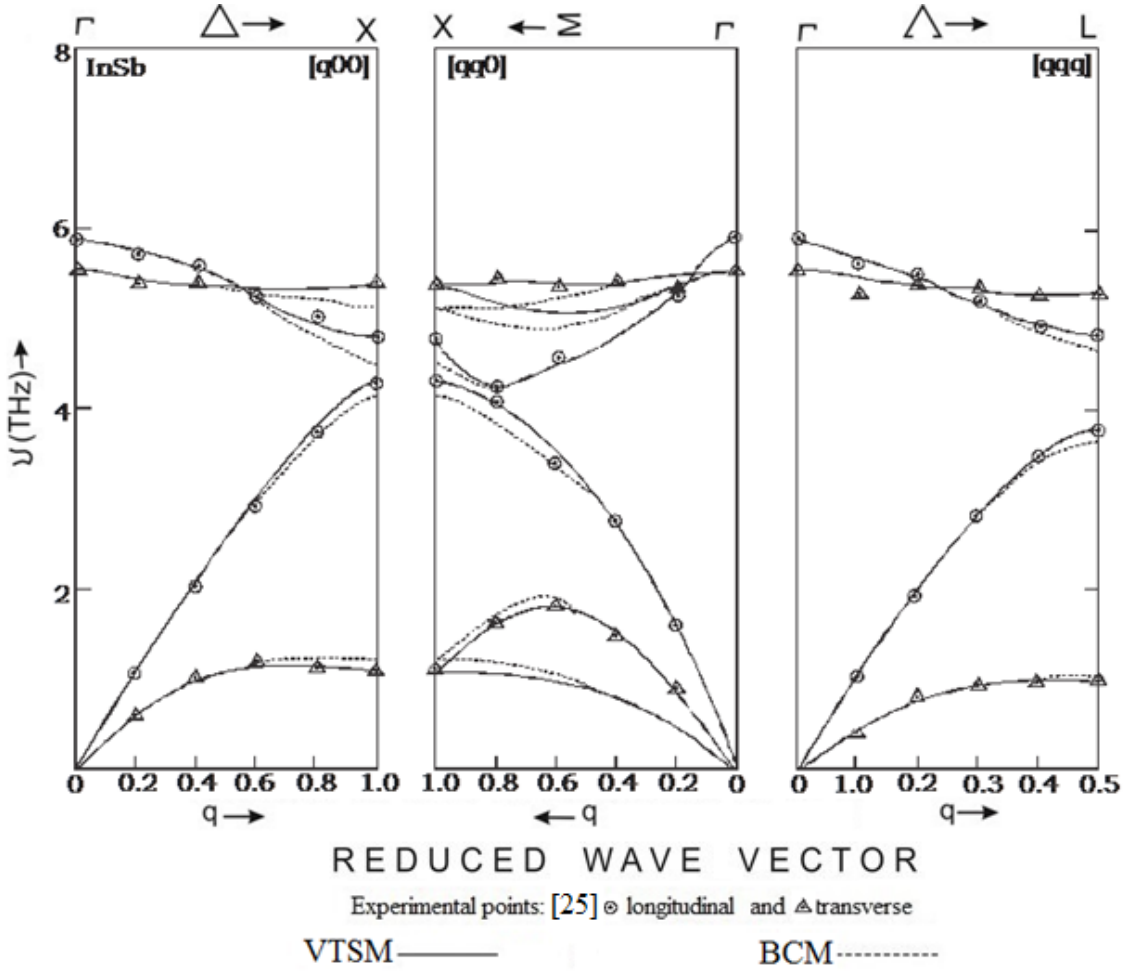

Figure 1. Phonon dispersion curves for InSb

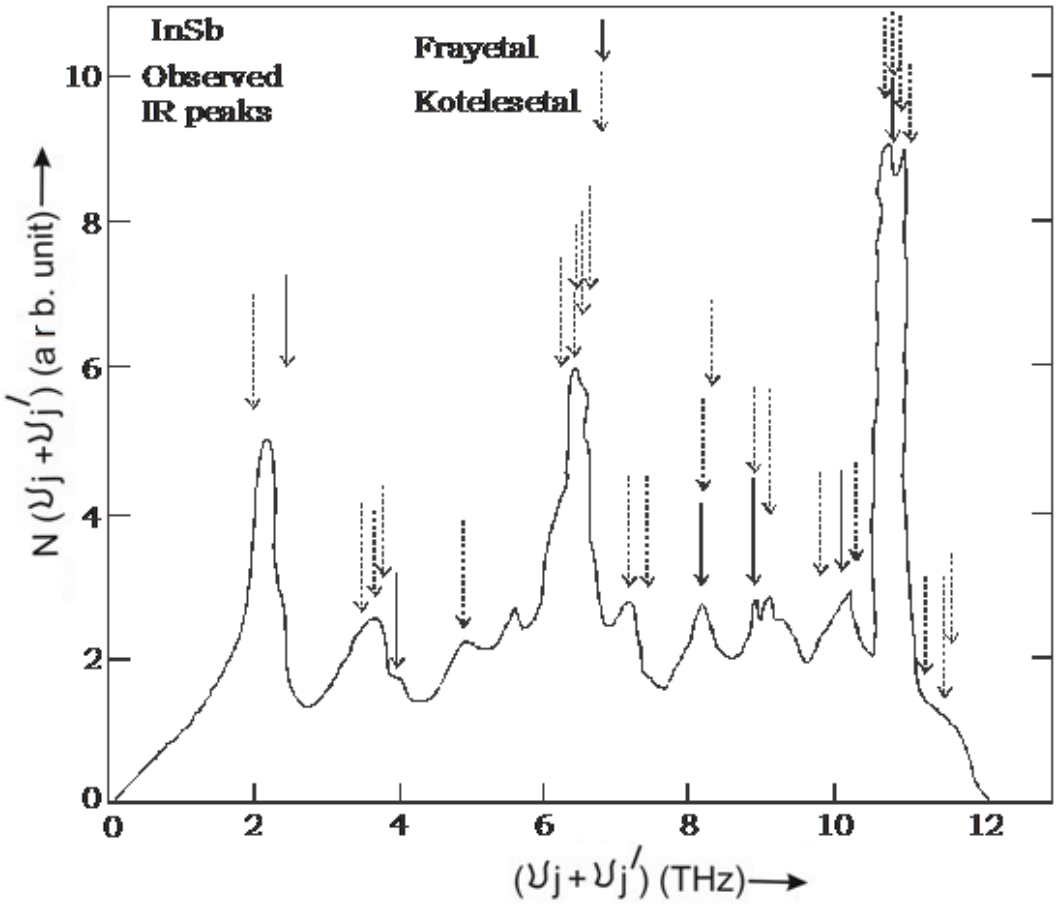

Figure 2. Combined density of states curve for InSb

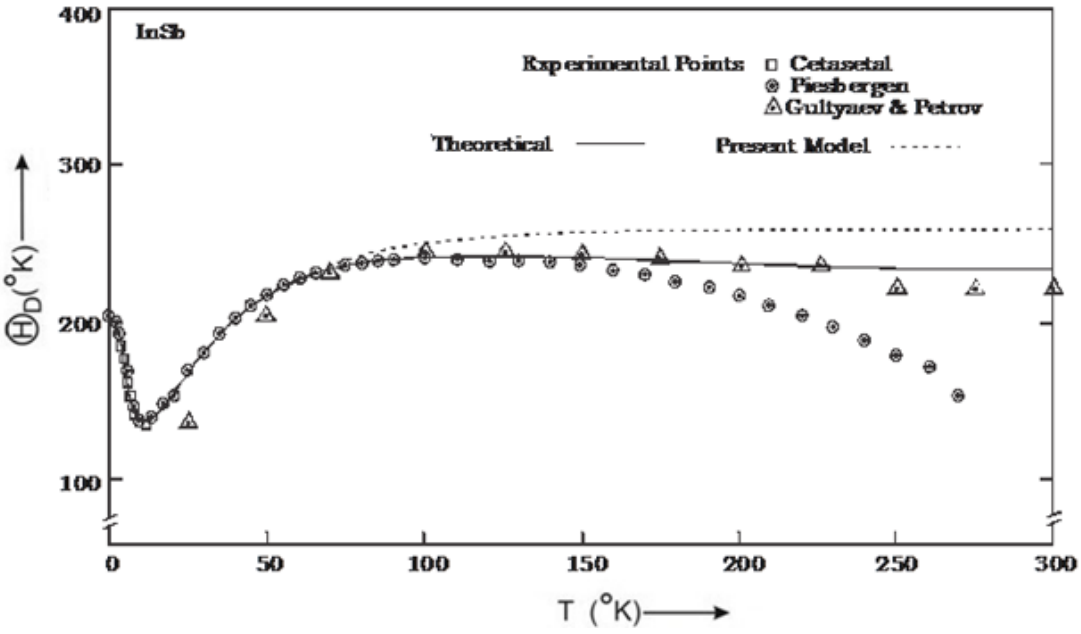

Figure 3. Debye characteristics temperatures Θ_D (°K) as a function of temperature T for InSb

The complete phonon spectra were used to compute the combined density of states CDS, $N(\upsilon_j+\upsilon_j)$ corresponding to the sum modes $(\upsilon_j+\upsilon_j)$ following procedure of Smart et al. [46]. A histogram between $N(\upsilon_j+\upsilon_j)$ and $(\upsilon_j+\upsilon_j)$ has been plotted and smoothed out as shown in Figure 2. These curves show well defined peaks which correspond to two-phonon IR spectra. These CDS peaks have been compared with the assignments calculated and shown in Table 3. The Debye temperature variation for InSb measured from [16,29,30,31,32] and those calculated by us using VTSM has been compared in Figure 3. The measured values of TOEC by Sadao [28] shown in Table 4. The measured values of pressure derivatives of SOEC by Peresada [47] have also been calculated us compared with these calculated by Ford et al. [48] in Table 5.

3. Results and Discussion

3.1. Phonon Dispersion Curves

From Figure 1, our phonon dispersion curves for InSb agree well with measured data reported by Price et al. [20]. It is evident from PDC that our predictions using present model VTSM are better than those by using BCM [25]. Our model has successfully explained the dispersion of phonons along the three high symmetry directions. From Figure 1 and Table 6, it is clear that: there are deviations of 5.26% along LO(X), 2.98% along TO(X), 1.16% along LA(X), 5.36% along TA(X), 1.87% along LO(L), zero% along TO(L), 3.94% along LA(L), 5.10% along TA(L) and 0.57% along LO(Δ), 1.72% along LA(Δ), zero% along TA(Δ) from experimental results. From BCM, deviations are 5.26% along LO(X), 4.27% along TO(X), 1.16% along LA(X), 7.14% along TA(X), 2.49% along LO(L), 0.19% along TO(L), 4.20% along LA(L), 7.14% along TA(L) and 0.95% along LO(Δ), 1.72% along LA(Δ), zero% along TA(Δ). From Table 6 it is clear that VTSM has very small deviation from experimental data. Our model, VTSM has 5.26% along LO(X), 5.36% along TA(X) and 5.10% along TA(L) improvement over BCM due to inclusion of TBI and VDWI coefficients. Thus, our VTSM model has better agreement with experimental data over BCM [25].

3.2. Combined Density of States

The present model is capable to predict the two phonon IR spectra [33,34]. The results of these investigations for CDS peaks have been presented in Figure 2. The theoretical peaks are in good agreement with both observed IR spectra for InSb. The assignments made by the critical point analysis have been shown in Table 3. The interpretation of IR spectra achieved from both CDS approach and critical point analysis is quite satisfactory. This explains that there is an excellent agreement between experimental data and our theoretical results.

Table 1. Input data and model parameters for InSb [C_{ij} and B (in 10^{11} dyne/cm^2), υ (in THz), r_0 (in 10^{-8} cm),α_i (in 10^{-24} cm^3), b (in 10^{-12} erg), ρ (in 10^{-8} cm)]

Input Data		Model Parameters	
Properties	Values	Parameters	Values
C_{11}	6.67[a]	b	1.790
C_{12}	3.65[a]	ρ	0.576
C_{44}	3.02[a]	$f(r_0)$	-0.260
B	4.51[b]	$r_0 f'(r_0)$	1.263
r_0	2.80[b]	A_{12}	15.199
υ_{LO} (Γ)	5.90[c]	B_{12}	-8.052
υ_{TO} (Γ)	5.54[c]	A_{11}	50.731
υ_{TO} (X)	5.38[c]	B_{11}	-12.341
υ_{TA} (X)	1.12[c]	A_{22}	–8.434
υ_{LO} (L)	4.82[c]	B_{22}	–42.125
υ_{LA} (L)	3.81[c]	d_1	0.219
α_1	0.22[d]	d_2	3.843
α_2	13.25[d]	Y_1	–0.476
ε_0	17.88[e]	Y_2	–1.633

[a]-(Slutsky [39]); [b]- (Banerjee [16]); [c]- (Price [20]); [d]- (Kunc et al. [40])]); [e]- (Hass [41])

Table 2. van der Waal's Interaction Coefficients for InSb (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_{+-}	956
C_{++}	431
C_{--}	2286
d_{+-}	748
d_{++}	227
d_{--}	2067
C	5200
D	3341

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

CDS Peaks (cm^{-1})	I.R Active			
	Observed I. R. Peaks		Present Study	
	Exp. [33]	[34]	Values (cm^{-1})	Assignments
73	83	-	80	2TA (Δ)
87	84-87	86	80	2TA (Δ)
-	115	-	-	-
-	117	-	-	-
134	124	134	137	LA + TA (Δ)
-	127	-	-	-
163	161	-	-	-
190	-	-	193	2LA(Δ)
205	208	-	-	-
212	211	-	-	-
-	214	-	213	TO + TA (L)
-	214	-	213	TO + TA (Δ)
218	219	-	217	LO + TA (L)
-	220	-	-	-
-	225	-	-	-
240	240	-	-	-
-	246	-	-	-
-	-	-	267	TO + LA (L)
270	-	-	270	TO + LA (Δ)
-	-	-	-	LO + LA (L)
-	273	274	273	LO + LA (Δ)
-	278	-	-	-
296	299	297	-	-
301	305	-	-	-
-	320	-	-	-
-	322	-	-	-
-	326	-	-	-
338	-	336	-	-
-	345	-	346	2TO (Δ)
-	349	-	350	LO + TO (Δ)
357	356	-	353	2LO (Δ)
-	359	361	-	-
-	363	-	-	-
-	367	-	-	-
-	370	-	-	-
-	375	-	-	-
-	384-388	-	-	-

Table 4. Third Order Elastic Constants (in the unit of 10^{11}dyne/cm^2) for InSb

Property	Present Study	Experimental Results [28]
C_{111}	−3.79	−3.56
C_{112}	−2.54	−2.66
C_{123}	−0.92	−1.00
C_{144}	+0.12	+0.16
C_{166}	−1.24	−1.39
C_{456}	−0.015	−0.004

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

Properties	Values		
	Present Study	Experimental [47]	Other [48]
dK'/dP	3.94	4.58	4.19
dS'/dP	0.53	0.47	1.23
dC'$_{44}$/dP	0.42	0.47	1.23

Table 6. Comparison of frequencies from various sources (X and L points) for InSb

Expt. [20] (THz)	BCM [25]			VTSM (Present Study)			% Improvement Over BCM (a ~ b)
	Value (THz)	(±) Deviation	% (a)	Value (THz)	(±) Deviation	% (b)	
4.75	4.50	0.25	5.26	4.75	0.00	0.00	5.26
5.38	5.15	0.23	4.27	5.30	0.08	1.49	2.98
4.30	4.25	0.05	1.16	4.30	0.00	0.00	1.16
1.12	1.20	0.08	7.14	1.10	0.02	1.78	5.36

3.3. Third Order Elastic Constants (TOEC), Pressure Derivatives of Second Order Elastic Constants (SOEC)

Our calculations on TOEC are reported in Table 4 and compared with measured data of Sadao [28] on TOEC of InSb. Further, pressure derivatives of SOEC for InSb have also been compared with the calculated results of Ford et al. [48] and measured data of Peresada [47] as shown in Table 5. The results are in good agreement.

3.4. Debye Temperature Variation

From Figure 3, our study shows a better agreement with the measured data of Banerjee, Gultyaev, Cetas, Piesbergen and Passler [16,29,30,31,32] and the theoretical results reported by Rajput and Browne [45] using BCM. To conclude, we can say that our present model gives a better interpretation of the Debye temperatures variation for InSb.

4. Conclusion

The inclusion of VDWI with TBI has influenced both the optical branches and the acoustic branches. Another striking feature of present model is the excellent reproduction of almost all branches. Hence the prediction of PDC for InSb using VTSM may be considered more satisfactory than from other models BCM [45]. The basic aim of the study of two phonon IR spectra is to correlate the neutron scattering and optical measured data of InSb. In this paper, we have systematically reported phonon dispersion curves, combined density of states, Debye temperature variation and a part of harmonic and anharmonic properties of InSb. On the basis of overall discussion, it is concluded that our VTSM is adequately capable of describing the crystal dynamics of InSb. This model has also been applied equally well to study the crystal dynamics of other compound of this group InP and InAs.

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