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Phonon Properties of Various Phases of Gallium Nitrides

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Abstract: ***The group-III nitrides are the most fascinating materials in these days due to their wide and direct band gap which make them incomparable candidate for applications in LDs, LEDs and optoelectronic devices. The significant features of these materials like short bond length, hardness, high thermal conductivity, low compressibility and high melting point makes them valuable for high frequency as well for high power electronic devices at extreme temperature. It is also predicted that GaN is promising candidate for spintronic application and high power semiconductor devices containing GaN can operate at high voltage. In spite of significant technological achievements only reserved effort has been made to examine the phonons of GaN. The phonon mode study is important for dynamical, thermo dynamical and other structural properties. Furthermore electron transport and non radiative electron relaxation process dependes upon excitations of phonons. So phonon properties are the most desired properties to study. Hence in this study it is decided to study the phonon properties of GaN using de Launey angular force constant model. The results obtained at zone centre are in better agreement with experimental results. The phonon dispersion has been investigated throughout the Brillion zone and hence phonon density of states and variation of specific heat with temperature has been obtained for both phases i,e, cubic and wurtzite phase of BN.***

I. INTRODUCTION

Group-III nitrides with direct and large band gap are suitable for sensors, low dimension structure and high-frequency devices (Alves et al., 1999; Haboeck et al., 2003) and can also be used in hostile environments. The group III-nitride devices can work at much higher temperatures and have large piezoelectric constants. GaN show some exceptional properties as its direct band gap and low sensitivity make it suitable for use in bright light emitting diodes and solar cell arrays for satellite. GaN based electronic devices has the potential to reduce energy expenditure for power transmission utilities. It is best suitable for light emission in blue and ultraviolet range. It also show ferromagnetic character at room temperature when strongly doped with manganese. It is also predicted that this material is promising candidate for spintronic application (Gebicki et al., 2008). High power semiconductor devices containing GaN can operate at high voltage, so that power loss is 80% less than that of silicon, moreover switching speed is very high. GaN based transistors perform better than silicon transistors in high temperature and high power electronic devices (Lee S. et al., 2011). The phonon properties are the most important properties as phonon excitations provide us information about the nature of inter atomic forces in crystal, which leads to an understanding of bonding and structural properties of compounds. But till the detailed and accurate information of vibrational spectra of GaN is missing. Experimental studies at higher pressure and temperature range are often quite limited and precise models are of utmost importance. So there has been a emergent interest in developing computational models to recognize and calculate the structural and dynamical properties of these materials. The phonon properties of were studied theoretically in past with the use of empirical methods like rigid ion model, ab initio calculation and Keating model do not give the physical clarity (Tutuncu e al, 2000, 2002). The short range de Launey angular force (DAF) model has produced the admirable lattice dynamical way out as it involves interaction of many particles through angular force. So in this study it has been decided to investigate phonon properties of both the phases of GaN using de Launey angular force constant model.

II. METHODOLOGY

In this study to obtain phonon dispersion curve and phonon density of state of GaN, de Launey angular force constant model has been used. This model assumes that atoms are vibrating with small amplitude and amplitude is so small that only elastic force is involved between these atoms and Hooke's law is supposed to be obeyed. This model consider two types of interatomic interactions: Central force and angular force. The de Launey force constant model involves interactions with its neighbors but this interaction reduces suddenly as the interatomic distance increases. Hence Interatomic interaction up to second nearest neighbors is considered and hence two force constants are involved for both central and angular interactions. The two involved constants α_1 and

α_2 represent central interaction while force constants α_1' and α_2' represent angular interactions of nearest and second nearest neighbors respectively. The non central restoring force acting on o due to i is given by,

$$F_i = -\alpha'(s_0 - s_i) - (\alpha - \alpha')\left[\hat{\zeta}_i X(s_0 - s_i)\right] X \hat{\zeta}_i$$

Using components of the non central forces the obtained secular determinant is of the form as given below.

$$\left[D_{ij}(q) - M\omega^2 I\right] = 0$$

Where D_{ij} are the elements of the dynamical matrix, i, j = 1, 2, 3 and I is the unit matrix.

Cubic structure has two atoms per unit cell hence a dynamical matrix of (6x6) has been established. The dynamical matrix is solved at zone centre (ZC) and along (q 0 0) to obtain the relation between force constants, frequency and elastic constants. The relations thus obtained are as given below.

$$\frac{4}{3}(\alpha_1 + 2\alpha_1') = \left[\frac{m_1 m_2}{(2m_1 + m_2)}\right]\omega_0^2$$

$$aC_{11} = \frac{1}{3}(\alpha_1 + 2\alpha_1') + 4(\alpha_2 + \alpha_2')$$

$$aC_{12} = \frac{1}{3}(\alpha_1 - 4\alpha_1') + 2(\alpha_2 - 5\alpha_2')$$

$$aC_{44} = \frac{1}{3}(\alpha_1 + 2\alpha_1') + 2(\alpha_2 + 3\alpha_2') - \frac{\left((\alpha_1 - \alpha_1')^2\right)}{(3(\alpha_2 + 2\alpha_1'))}$$

Here m_1 is the mass B atom and m_2 being mass of N atom. C_{11}, C_{12} and C_{44} are the elastic constants and a is the lattice parameter. By using ZC phonon frequency (Huan 2008; Alvesa 2002) experimental values of the elastic constants as given by (Shervin 1991; Marmalyuk 1998) and as input parameters the force constant has been calculated and are given in table I.

The wurtzite structure has four atoms per unit cell hence a dynamical matrix of (12x12) has been established. The dynamical matrix of (12 x 12) thus established is solved at the zone center to obtain relation between some key vibrational frequencies and force constants. By solving the (12x12) dynamical matrix the following relations between force constants and some important vibrational frequencies are obtained.

$$\frac{4}{3}(\alpha_1 + 2\alpha_1') = \frac{m_1 m_2}{m_1 + m_2}\omega_{E_1(TO)}^2$$

$$\frac{4}{3}(\alpha_1 + 2\alpha_1') + 2(4\alpha_2 + 2\alpha_2') = m_2\omega_{A_1(TO)}^2$$

$$4(\alpha_2^2 + 25(\alpha_2')^2 + 10\alpha_2\alpha_2' - \alpha_1^2) + \frac{16}{3}(\alpha_1 + 2\alpha_1')(\alpha_2 + 5\alpha_2' + \alpha_1) - \left(\frac{4}{3}(\alpha_1 + 2\alpha_1') + 2\alpha_1 + 10\alpha_2'\right)(m_1 + m_2)\omega_{E_2^h}^2 + m_1 m_2 \omega_{E_2^h}^4 = 0$$

$$\alpha_2 + 5\alpha_2' + \alpha_1' = \frac{m_1}{2}\omega_{E_2^l}^2$$

Here m_1 and m_2 are the mass of X (Al, Ga, B and In) and N atom respectively. By using the experimental values of the zone centre frequencies, m_1 and m_2 as the input parameter the above equations are solved to calculate force constants. The force constants thus obtained are given in table I.

TABLEI: Calculated Force Constants For Cubic Phase Of Gan

Phase	Force constant (10^4 dyne cm^{-1})				Lattice constants (Å)	
	α_1	α_1'	α_2	α_2'	a	c
Cubic	23.78	3.225	4.335	0.55	3.62	-
Wurtzite	19.385	5.3716	6.3666	-1.7308	2.56	4.23

III. SYMMETRY PROPERTIES

The cubic BN has two atoms in a unit cell occupying O_h sites with space group $F\bar{4}3m$ and are contributing to the normal modes at symmetry points of the Brillouin zone. Accordingly at Γ point, atomic vibrations can be represented as

$$\Gamma = 2T_2$$

$$\Gamma_{ac} = T_2 \quad \Gamma_{opt} = T_2$$

T_2 represent the triply degenerate modes.

The wurtzite phase has 4 atoms per unit cell with space group C_{6v}^4 ($P6_3mc$) with two formula units per primitive cell (Tutuncu et al., 2000; Dutta et al., 2001). Atoms are occupying C_{3v} sites and in the primitive cell contribute to the normal modes at symmetry points of the Brillouin zone (BZ). Accordingly at zone centre atomic vibrations can be represented as

$$\Gamma = \Gamma_{ac} + \Gamma_{opt} = 2(A_1 + B_1 + E_1 + E_2)$$

$$\Gamma_{ac} = A_1 + E_1 \qquad \Gamma_{opt} = A_1 + 2B_1 + E_1 + 2E_2$$

The E_2 modes are only Raman active, both E_1 and A_1 are both Raman and IR active while B_1 modes are silent (Tutuncu et al, 2000).

IV. RESULTS AND DISCUSSIONS

The digonalization of (6x6) and (12x12) dynamical matrics for cubic and wurtzite structure respectively gives us the phonon frequencies and thus obtained phonon frequencies along with other theoretical results and few available experimental phonon frequencies at ZC are given for comparision in table II.

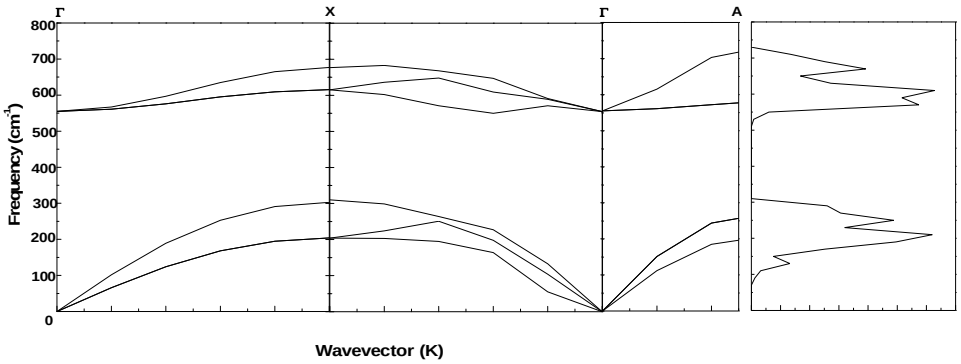
TABLE 3.2: Zone Centre Phonon Frequencies (Cm^{-1}) Of Gan

Phase	Phonon modes	This work	Other theoretical results[a,b]	Other theoretical results[c,d]	Experimental results[e,f]
Wurtzite	E_2(low)	177	147	136	145
	B_1(low)	239	331	330	
	A_1(TO)	533	536	531	533
	E_1(TO)	561	534	555	561
	E_2(high)	570	559	564	570
	B_1(high)	561	710	684	
Cubic	TO	555	557	555	555

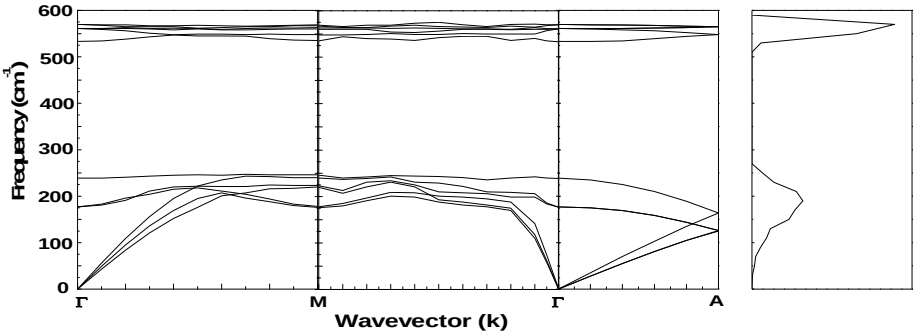
a = Zhang et al., (2013), b= Dario et al., 2010, c = Pereira et al., (2003), d = Karch et al., 1997, e = Tutuncu et al., (2000) f = = Bechstedt F et al., 2005.

It is observed that obtained phonon frequency for cubic phase match wth the experimental frequency while for wurtzite structure E_1(TO), A_1(TO) and E_2 (high) mode show no deviation from experimental results while a significant deviation is observed in case of the results obtained by other theoretical results. E_2(low) mode show more deviation (11%) than that of the other theoretical results but overall the results of this work are in better agreement with the experimental results at ZC. Now both the dynamical matrices are diagonalized along the different symmetry directions to obtain phonon dispersion curve. It is found for wurtzite phase that out of nine optical modes the doubly degenerate E_2 modes (177 cm^{-1} and 570 cm^{-1}) are Raman active while the A_1 (533 cm^{-1}) and doubly degenerate E_1 (561 cm^{-1}) modes are both Raman and infrared active. The B_1 modes (239 cm^{-1} and 561 cm^{-1}) are silent. It is observed for both phases that contribution of nitrogen atom is more towards higher optical phonon frequencies while contribution of Ga-atom is more towards lower optical phonon frequencies, which is due to heavier mass as Ga atom than N atom. But for B_1 (low) mode the contribution of nitrogen atom is negligible while for B_1 (high) mode the contribution of Ga is negligible**.** The difference of masses

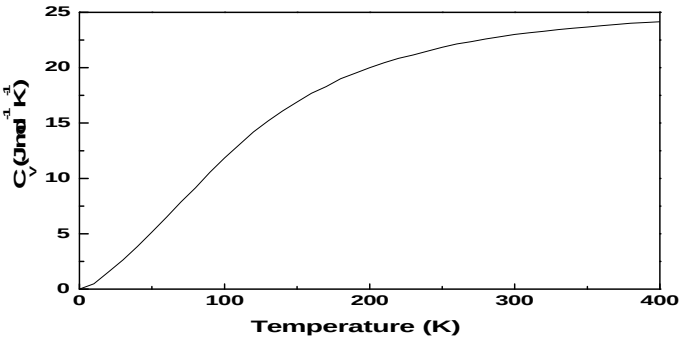
of cation (Ga) and mass of anion (N) results in gap between acoustic and optical branches which is more for wurtzite phase as compared to cubic phase. The phonon density of state for wurtzite phase of GaN show two sharp peaks at 570 cm^{-1} and at 190 cm^{-1} which corresponds to upper lying optical modes and combination of acoustical modes, B_1 (low) and E_2 (low) modes along with a small flattened peak. While for cubic phase the sharp peaks observed at at 610 cm^{-1} and 570 cm^{-1} corresponds to optical region while sharp peaks observed at 220 cm^{-1} and 280 cm^{-1} corresponds to acoustical region.



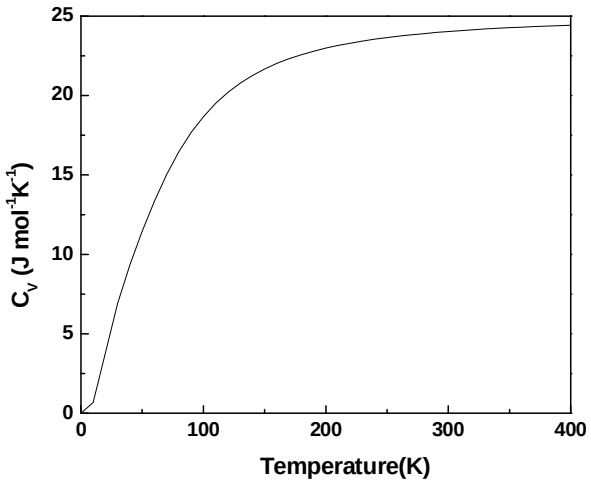
Graph 1 Phonon dispersion curve and phonon density of states for cubic phase



Graph 2 Phonon dispersion curve and phonon density of states for cubic phase



Graph 3 Variation of specific heat with temperature for cubic phase



Graph 4 Variation of specific heat with temperature for wurtzite phase

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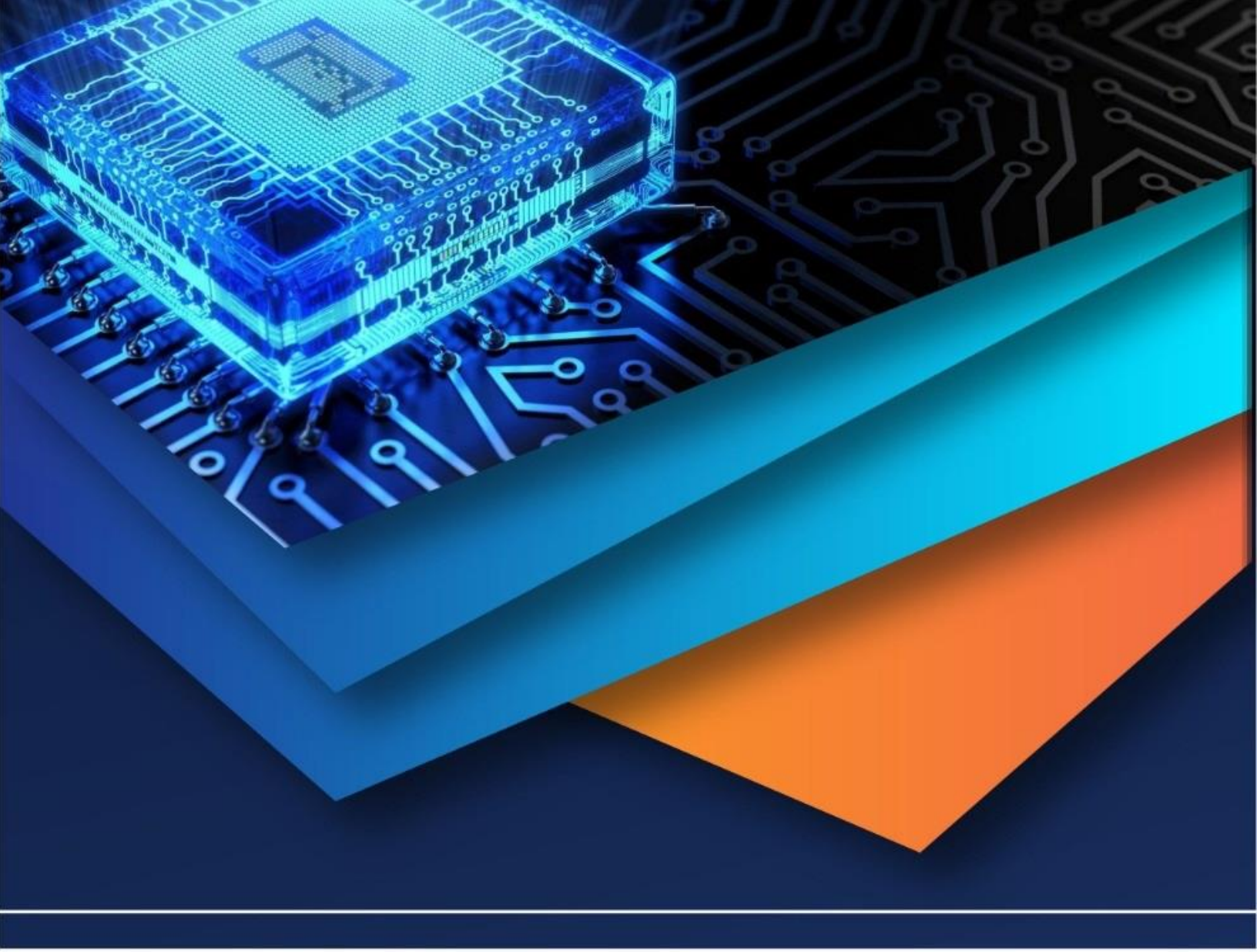

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