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Vibrational Properties of Wurtzite Phase of AIN and GAN

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Abstract: ***The group-III nitrides are the semiconductors of utmost interest due to their fascinating properties and their performance under eminent conditions of temperature. Phonons play an important role in the electron transport, electron relaxation process, dynamical, thermodynamical properties, and many more properties. We have calculated the Phonon dispersion throughout the Brillouin zone, phonon density of state, specific heat and anisotropy for wurtzite phase of AlN and GaN. de Launey angular force constant model has been used in this study as this model includes many body interactions and is also better option for structures having partially covalent character. The calculated results are in good agreement with existing experimental data at zone centre and predict phonon dispersion throughout the Brillouin zone. The calculated specific heat also found to be obeying well known relation*** $C_v = 3R$***.***
Keywords: Lattice dynamics, phonons, Phonon Dispersion Curve, Specific heat and PDOS

I. INTRODUCTION

The nitride based semiconductors have attracted a considerable attention in last two decades due to their distinguished properties especially direct and wide band energy gap. The band gap of group-III nitrides enable these materials useful for optoelectronic devices, LED's, detectors operating in UV and visible spectrum and laser diodes. The important features of these materials like hardness, low compressibility, short bond length, high melting point and high thermal conductivity make them useful for high frequency and high power electronic device at extreme temperature [1, 2, 4]. These materials with large piezoelectric constant are highly significant to be used as sensors, low dimensional structures and high frequency devices [3]. The phonon study of the materials is the key for dynamical, optical transitions due to phonons, structural and thermodynamical properties. Moreover non radiative electron relaxation process and electronic transport are also influenced by excitations of phonons [5]. So the most desired properties are phonon dispersion curve and phonon density of state. The group-III nitrides have two crystallographic phases Zinc blende (cubic) and wurtzite phase. The Cubic phase has high symmetry but the wurtzite phase is considered as the most stable structure for nitride [6] and also can be used under ambient conditions.

The Raman scattering and inelastic neutron scattering are mostly used to study phonons experimentally in bulk material. The most experimental studies have been investigated the phonon modes at zone centre using first order Raman scattering [7]. Most of the theoretical studies are calculating electronic band structure. The vibrational properties of these materials are studied by using number of empirical methods like rigid ion model, valence force model, ab intio calculation and keating model etc. lacks physical clarity [8,9,10]. The de Launey angular force constant model gives an excellent lattice dynamical solution by involving many particle interactions. Recently Zhang et al. [2] and Fu et al. [1] have studied the phonon dispersion curve and density of states by generalized gradient approximation (GGA) and local density approximation (LDA). The calculated results by both methods do not agree with the each other. Moreover for AlN results also significant deviation from experimental results. The specific heat has been calculated by wei guang-hong et. al.[7] in temperature range (0-200K) and by L.S Pereira et. al. [6] in temperature range (0-100K).

But according to best of our knowledge only selected phonon modes at zone centre had been studied experimentally using first order Raman scattering. The full vibrational spectra can be studied by second order Raman scattering but that has not been reported. So we have decided for the Lattice dynamical study of wurtzite phase of AlN and GaN. We have obtained phonon dispersion curve and phonon density of states of AlN and GaN. The results show an excellent agreement with available experimental data at zone centre and zone boundary. Also specific heat of these materials have been calculated in temperature range (0-400K), which obey debye's law.

II. METHODOLOGY

In present study to formulate phonon dispersion curve, phonon density of state and specific heat of AlN and GaN. We have used de Launey angular force (DAF) constant model. This model worked on basis of Born-Von karman theory. In this theory the atoms in

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crystal structure are assumed to be exerting elastic force on each other and are oscillating with small amplitude. Oscillations are so small that Hook's law is supposed to be obeyed. This model include two types of interaction between atoms (1) Central force which acts on line joining the centers of the atoms and (2) angular force which depends upon angle between line joining equilibrium position and line joining the moving atoms. This system has benefit of incorporating interaction between many bodies through angular force and is suitable for the materials with partially covalent character. We have consider the interaction upto second nearest neighbors as this model based on short range forces and magnitude of the forces generally diminishes after second neighbor interatomic interaction. For central force, the force constants are α_1 for Al(Ga)-N and α_2 for Al (Ga)-Al (Ga), while for angular force the force constants are constant α'_1 for Al(Ga)-N and α'_2 for Al (Ga)-Al (Ga). The combined interaction of central and angular force is called non-central force and is given by

$$\vec{F} = -\alpha'\left(\vec{S}_0 - \vec{S}_i\right) - (\alpha - \alpha')(\hat{\zeta}_i)[\hat{\zeta}_i.\left(\vec{S}_0 - \vec{S}_i\right)] \quad \text{---------- (1)}$$

Where S_o and S_i are the displacements of the reference atom and ith atom

$\hat{\zeta}_i$ is the unit vector along the line joining the reference atom to the ith atom.

By solving the equation 1 for each atom along three coordinate axis results in secular eigen value equation given as

$$[d(k) - m\omega^2 I] = 0 \text{ ---------- (2)}$$

In our calculation for three dimensional lattice primitive cell contains four independent atoms, hence we get a 12 x 12 matrix whose solution yields 3 acoustical and 9 optical modes. The matrix is solved along long wavelength limit and force constants have been calculated.

Table 1. The Obtained Force Constants and Experimental Values of Lattice Constants [16]

S.No	Element	Force constant(10^4 dyne cm^{-1})				Lattice constants (Å)	
		α_1	α'_1	α_2	α'_2	a	c
1	AlN	10.525	2.8951	0.0933	0.2703	3.11	4.98
2	GaN	11.953	3.3197	0.7136	0.2103	3.19	5.20

By using the obtained force constant the frequency is calculated at zone centre, zone boundary and in the brillioun zone which is shown in graph 1 and graph 2 for AlN and GaN respectively. To calculate phonon density of state we use sampling method. In this method we solve the matrix at 84 point with suitable statistical weight, which results in the formation of mesh in irreducible section of first BZ. By sorting out different frequencies, frequency distribution function g(ν) has been evaluated.

The specific heat at constant volume has been calculated from vibrational spectra using Blackman's sampling technique and according to it specific heat C_V is given by

$$C_V = k \int_0^\infty x^2 e^x g(\nu) d\nu / (e^x-1)^2 \quad \text{--------(3)}$$

Here x = hν/kT, T is temperature, k is Boltzmann's constant and h being the Planck's constant. Specific heat C_V can be calculated from the frequency spectrum. In this presentation the frequency spectrum is obtained in suitable different frequency intervals which reduces the equation (3) to

$$C_V = \sum C_V(\nu) g(\nu)/12000 \text{ -------(4)}$$

All the atoms of the are supposed to be vibrating with same frequency ν and $C_v(\nu)$ is specific heat for the system. Using Einstein's quantum theory the specific heat corresponding to each (hν/kT) is determined. According to this theory, the average energy of an oscillator is given by $h\nu/(e^x - 1)$. Accordingly the energy of a gram atom of the solid consisting of N atoms is $U = 3N\, h\nu/(e^x - 1)$, We have then

$$C_v(\nu) = dU/dT = 3R\, x^2 e^x/(e^x-1)^2 \quad \text{----------(5)}$$

Using this expression $C_v(\nu)$ can be measured for different values of x. By using the value of $C_v(\nu)$, the average specific heat for wurtzite phase of AlN and GaN is calculated using equation (4). The specific heat is calculated for various temperatures ranging from 0K to 400K and is shown graphically in graph 3 and graph 4 for AlN and GaN respectively.

III. RESULT

As wurtzite crystal structure has 4 atoms per unit cell with space group C_{6v}^4 ($P6_3mc$) with two formula unit per primitive cell. All the atoms are occupying C_{3v} sites. All the atoms in the primitive cell contribute to the normal modes at symmetry poins of the BZ. As a result, we have

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

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

The E_2 are Raman active, A_1 and $E_1$are both Raman and IR active and the two B_1 modes are Raman as well IR silent.

Our calculation yields 12 modes, some of the modes degenerate at zone centre and at zone boundary. The phonon modes are studied in the Brillouin zone in this presentation and are shown in graph 1 and graph 2 respectively for AlN and GaN.

TABLE II The Comparison of Results with Theoretical Results and Experimental Results

		E2(low)	A1(TO)	E1(TO)	E2(high)	B1 (low)	B1 (high)
AlN	This Work	285	614	673	660	442	673
	Theory [2]	233	597	659	638	540	679
	Experiment[5]	252	614	673	660		
GaN	This Work	177	526	561	570	239	561
	Theory[2]	147	536	534	559	331	710
	Experiment[5]	145	533	561	570		

It can be clearly observed from table I that interatomic forces are stronger in AlN as compared to GaN as the values of the force constants for AlN are larger than GaN, this is because of smaller lattice constant of AlN as compared to GaN. Also the force between Al (Ga) and N given by force constant α_1 is strongest as compared to others. It has been observed that two regions are there in phonon dispersion curve one corresponds to acoustical mode and other to optical mode. The acoustical mode of both AlN and GaN shows more dispersion in comparison to optical mode. From the comparison of the phonon dispersion curve of both it has been observed that dispersion in AlN is more as compared to GaN in both acoustical and optical modes. The gap between optical and acoustical mode in case of GaN is more than AlN, this frequency gap is given by zone boundary phonons with Al (Ga) atom mass lower limit and N atom mass upper limit, hence larger the mass difference larger will be the frequency gap as the mass of Ga is more as compared to Al so gap is more for GaN. The band gap between optical and acoustical mode almost 275 cm^{-1} for GaN while for AlN is 150 cm^{-1}. Moreover the greatest frequency of optical phonon is more for AlN due to small cation mass. The E_1 (TO) and A_1(TO) splitting in case of AlN is more than GaN. The phonon density of states has also been obtained for both AlN and GaN In phonon density of states for AlN a sharp peak is observed corresponding to 673 E_1(TO) mode which is due to flatness of optical phonons in phonon dispersion curve while no such peaks observed corresponding to acoustical modes which is due to dispersion of acoustical mode, while in GaN one peak is observed corresponding to 561 E_1(TO) in optical region and, while small peaks are also observed for 285 and 177 E2(low) in acoustical region which is due to comparatively lesser dispersion. The band gap between acoustical and optical modes in PDOS increases with cation to anion mass ratio. The PDOS show that acoustical modes and optical modes are well separate in GaN while almost no gap in AlN. By using density of state Specific heat of AlN and GaN also has been found using Debye's Law in temperature range (0-400K). It is clear from the graph that specific heat increases rapidly at lower temperature and then rate of increase decreases continuously and almost becomes flat when the specific heat approaches 3R. The observations are in excellent agreement with existing results. We also have calculated the anisotropy of AlN and GaN. The anisotropy of wurtzite structure also causes the deviation in phonon modes is A-Γ and M-Γ direction.

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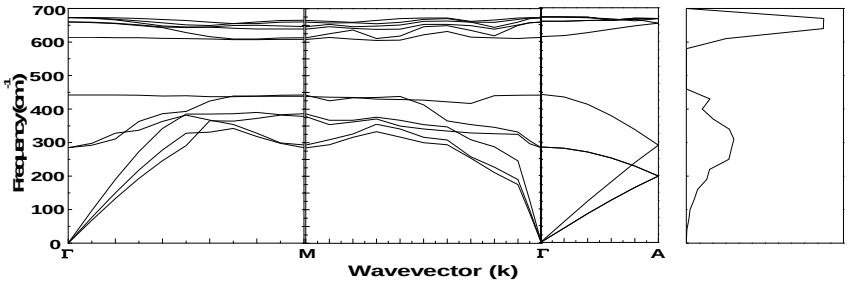
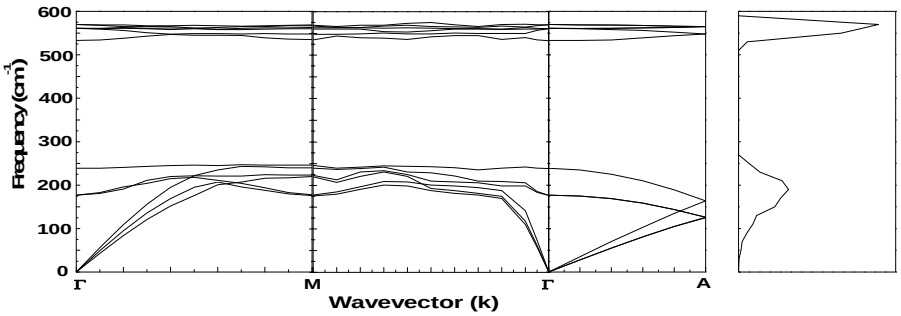
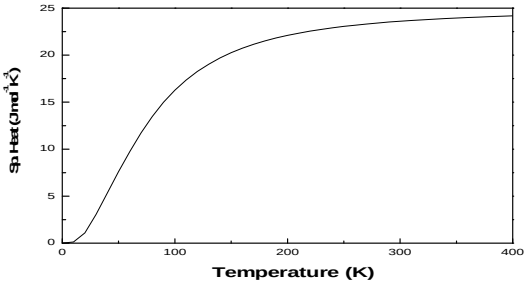


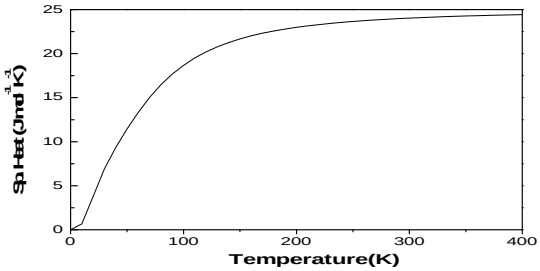
Graph I Phonon dispersion curve and phonon density of states of AlN



Graph II Phonon dispersion curve and phonon density of states of GaN



Graph III variation of Specific heat with temperature for AlN



Graph IV variation of Specific heat with temperature for GaN

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H Zhang et.al.[2] have studied the phonon dispersion and phonon density of states using LDA and GGA. J Q Fu et. al.[1] have studied the phonons of AlN using GGA and LDA. If we compare our results with the results of above mentioned theoretical results and experimental results at zone centre. Our result shows much better agreement with the experimental values with small deviation as compared to the existing results. The comparison of results with theoretical results [2,1] and experimental results [5] are given in table II. Specific heat capacity has also been found for AlN and GaN in temperature range (0-400 K) results shows an excellent agreement with Debye's law. So far specific heat has been observed by weiguang-hong et. al.[7] in temperature range (0-200) and by L.S Pereira [6] in temperature range (0-100k). So it is hoped that our calculated results for specific heat at higher temperature will be helpful for the researchers for reference in future research.

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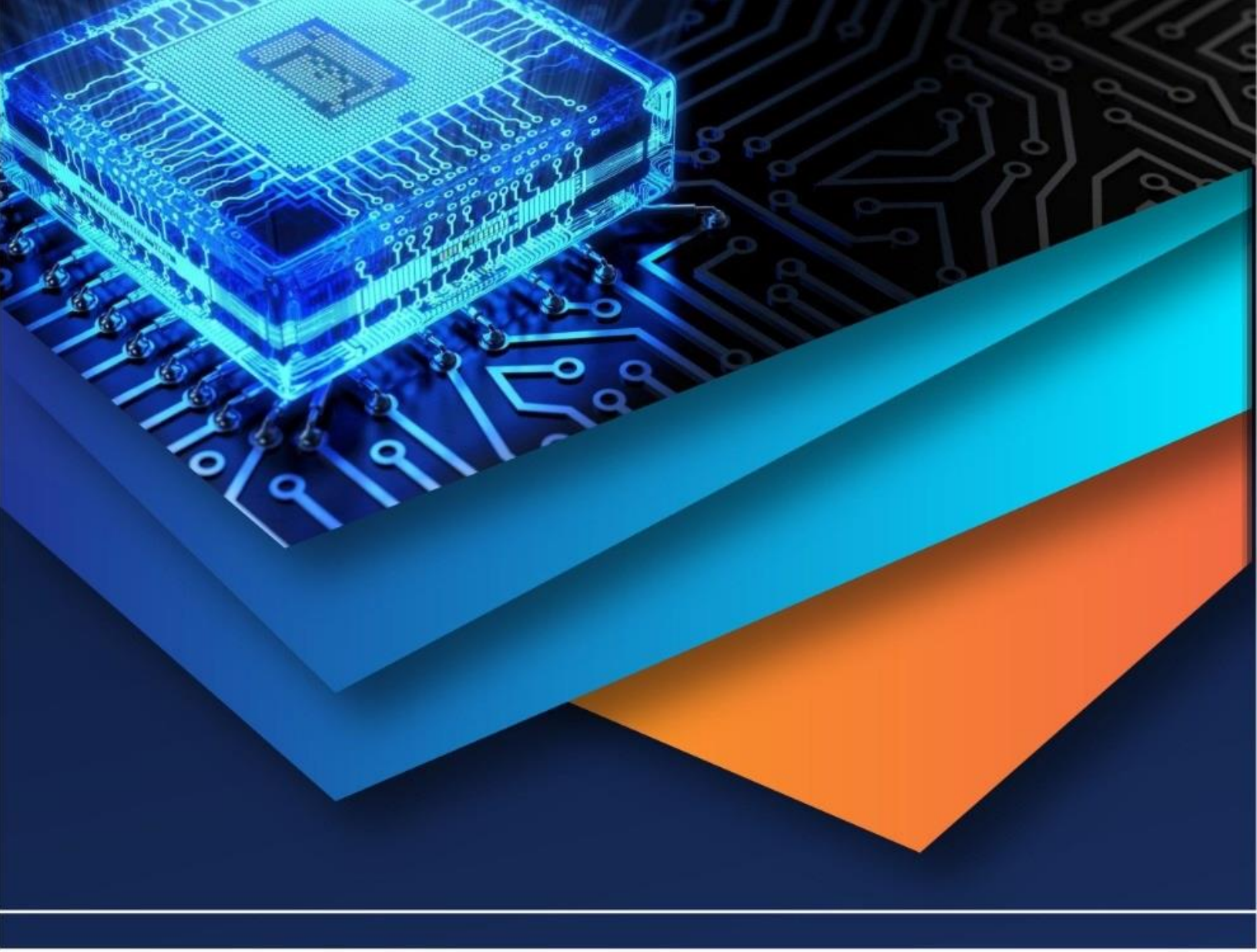

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