Dynamical Properties of Group-III Nitrides in Cubic Phase

Daljit Singh, M M Sinha

Abstract--We study the lattice dynamics of nitrides of Al, In, B and Ga in cubic phase using short range force constant model. Using this model we obtained the phonon dispersion curve, phonon density of states for group III Nitrides. The present results are compared will existing results and it is found that results show excellent agreement will existing results. The results are also verified by some existing facts.

Keywords-- Cubic phase, Dispersion relation, Density of States, force constant model, Lattice dynamics, phonons, III-Nitrides

1. INTRODUCTION

The group-III nitrides (AlN, BN, GaN and InN) and their alloys are significant materials for high- power, high-frequency, and high-temperature optoelectronic applications, so these are used to make light emitting and laser diodes[1] and high-power electronics (e.g. HEMTs) [2]. Most of their potential in these fields is because of wide band gaps. With alloy composition the band gap varies between 1.9 eVto 6.2 eV. The breakdown electric field strength of these materials is much larger than that of either Si or GaAs because of the large band gap energy of the III-nitride [3-5], also enabling, at least in principle, much higher maximum output power delivery in power amplifiers. These materials are also used for protective coating due to their hardness, high melting point and high thermal conductivity [6]. . Also group III-IV are most fascinating material for researchers due to its high melting point, high thermal conductivity and large bulk modules [7]. Due to their special features group-III nitrides have attracted a lot of attention in nanoscale science and technology in recent years [8]. Taken into account of its wide applications, we have studied lattice dynamics of cubic phase of nitrides in this presentation. The Lattice dynamics is basic to study of solid state and is described in terms of lattice vibration wave vector, frequency and polarization properties. The physical properties of solid, including the thermal, optical and electrical properties, are directly dependent upon the frequency-wave vector relationship called phonon dispersion relation. Phonon dispersion relation is the most important feature for the dynamics of atoms, crystal and is of special importance for solid state physics and material science.

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Phonon dispersion relations is useful to understand the excitations that crystal lattice can experience and for their thermal, optical and electric properties Phonon dispersion relations can be obtained by both computational and experimental determination. The interactions with the first-nearest-neighbor and second-nearest-neighbor atoms are characterized by central and noncentral angular forces [9, 10]. The theoretical treatment of the group-III nitrides have problem due to the extreme differences of mass between the cations and the nitrogen anion, in especially for GaN and InN. The extremely different atomic sizes and electronegativities cause considerable charge transfers between cations and anions and, hence, strongly ionic bonds [11].

Recently, the lattice dynamics of the zinc-blende and wurtzite phases of III-Nitrides has been studied using the ab initio pseudo potential method [17 -22] and an adiabatic bond –charge model [23-24]. Recently, the lattice dynamics of wurtzite AIN and GaN has been investigated by inelastic x-ray scattering [25-26].

But exact information about dynamical properties is still missing. As results of second order Raman scattering experiments about phonon modes along brillouin zone have not been reported [1]. Also this technique has limitation that it can measure only phonon with small wave vector [6]. Many researchers have studied phonon spectra of group – III nitrides by constructing an empirical model and then adjust force constant to match the experimental calculations. So these methods results in uncertainty to some extent [34].

The phonon frequency is fundamental characteristic of these crystals. It determines their thermal and optical properties including phonon assisted optical transition. Therefore a study of lattice dynamics of nitrides is not only of fundamental interest but result in a better understanding of structural parameter responsible for the efficiency of optical devices.

The objective of this paper is to apply a short range force constant model to obtain dynamical properties of the cubic phase of GaN, InN, AlN and BN and to give better results

as compared with previous calculations and missing information from experimental data in the literature.

2. THEORY

The III-V nitride materials exist in both hexagonal wurtizite and cubic zinc-blend structure [1]. However, devices with a zinc-blend structure would have considerable advantages. The cubic nitrides are expected to have higher mobility, due to the decrease of the phonon number for the higher symmetry structure. Therefore, information on the vibrational properties of these nitrides in cubic phase is strongly desirable. It is suggested that due to reduced phonon scattering in the high-symmetry crystals the electronic and thermal properties of zinc-blend (cubic) nitrides will be superior to those of the wurtzite materials. The cubic nitrides are also believed to be better suited for doping than the wurtzite[6]. Therefore, in the present study we have studied phonons of zinc-blend structure of AlN, BN, GaN and InN in phase by applying short range force constant model.

The zinc-blend structure consists of 2 identical interpenetrating face centred cubic lattices based on nitrogen atoms at (000) and Al(In,B,Ga) at(¼, ¼, ¼) in the cubic unit cell. The dispersion relation is given by the solution of the characteristic equation.

$$|D(k) - m\omega^2 I| = 0 \quad \text{----------(1)}$$

Where D(k) is a (6X6) dynamical matrix and I is a unit matrix. Here we have considered the entire interaction in AI(In ,B,Ga) and N consists of two parts: the ion-ion radial interaction in between the ions is known as central force and second is angular force. The central forces are assumed to act along the line joining the two neighbors. The angular force is due to de-launey and is referred to de-launey angular force constant model [26]. The angular force depends upon the angle which the line joining the moving atom to its neighbors makes with the equilibrium position of the line. In the present calculation α_1 and α_2 are taken as central force constants and $\alpha_{1'}$ and $\alpha_{2'}$ as angular force constants between atoms AI (In, B, Ga)- N and AI(In, B, Ga)-AI or N-N respectively. By considering these force constants a dynamical matrix D(k) of 6X6 is established. The dynamical matrix is solved at (0,0,0), (q,0,0) and (q,q,q)to obtain the relation of force constants with zone centre frequency and elastic constants. The relations thus obtained are given below,

$$4/3(\alpha_1 + 2\alpha_1') = [mM/(2m+M)]\omega_0^2 \quad \text{----------(2)}$$

$$aC_{11} = 1/3(\alpha_1 + 2\alpha_1') + 4(\alpha_2 + \alpha_2') \quad \text{----------(3)}$$

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

$$aC_{44} = 1/3(\alpha_1 + 2\alpha_1') + 2(\alpha_2 + 3\alpha_2') - \{(\alpha_1 - \alpha_1')^2\}/\{3(\alpha_2 + 2\alpha_1') \quad \text{----------(5)}$$

Here m the mass of X(X = Al, Ga, B or In) and M being the mass of N atoms. By using the following results as given in table I for zone centre phonon frequency [29-30] and elastic constants [31-32] to the above equations, the centre and angular force constants are calculated and are listed in table II.

TABLE I INPUT PARAMETERS

Compound	Zone centre phonon frequency (cm-1) 29,30]	Lattice parameter (A0) [29-30]	Elastic constant [31-32] (1011 dynes.cm-2)		
	ω0	A	C11	C12	C44
BN	1055	3.62	82	19	48
GaN	555	4.5	30.5	12.8	14.7
InN	489	4.98	21.7	10.1	10.4
AlN	655	4.38	32.8	13.9	13.3

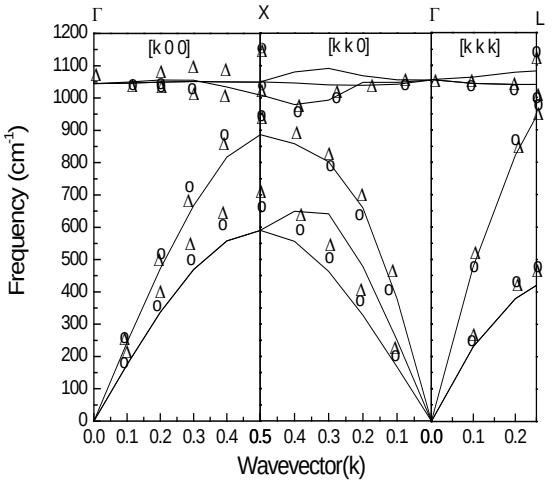
TABLE II CALCULATED FORCE CONSTANTS AND ZC FREQUENCY

Compound	Force constant (dyne cm-1)				ZC frequency (cm-1)
	α1	α1′	α2	α2′	ω0
BN	23.78	3.225	4.335	.55	1055
GaN	14.06	0.98	1.95	.15	555
InN	11.28	1.01	1.54	0.05	489
AlN	15.32	1.15	2.17	0.15	655

3. PHONON DISPERSION CURVES

The force constants thus obtained are used to solve the matrix in the symmetry direction (q, 0, 0), (q, q, 0) and (q, q, q). By using these force constants the phonon dispersion curve have been obtained.

In the present calculation the phonon dispersion curve in three symmetric directions have been obtained by using the calculated force constants. The calculated ZC phonon frequency is in excellent agreement for all group-III nitrides with experimental results [17,20,and9]. The phonon dispersion curve for BN, AlN, GaN and InN are shown in Fig. 1(a), Fig. 2(a), Fig. 3(a) and Fig. 4(a) respectively.



ig. 1(a) Solid line represents the obtained phonon dispersion curve. Triangles represent the results of Dario G et.al. (1) while circle represent the results of H M Tuttuncu et.al.(6)

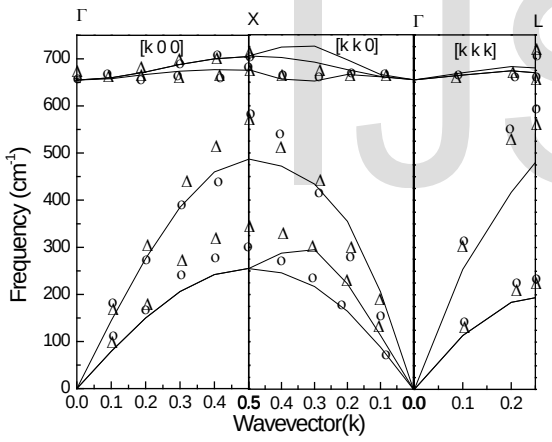


Fig. 2(a) Solid line represents the obtained phonon dispersion curve. Triangles represent the results of Dario G et.al. (1) circle represent the results of H M Tuttuncuet.al(6)

Same has been observed by H M Tutuncu et. Al. [6,23] and F Bechstedt et al [8]. The frequency gap for group-III nitrides decreases in the sequences InN - GaN - AlN - BN. It is also observed that interatomic interaction is maximum between B and N and is minimum for InN, It is due to the fact that interatomic interaction varies inversely proportional to the lattice constant [8].

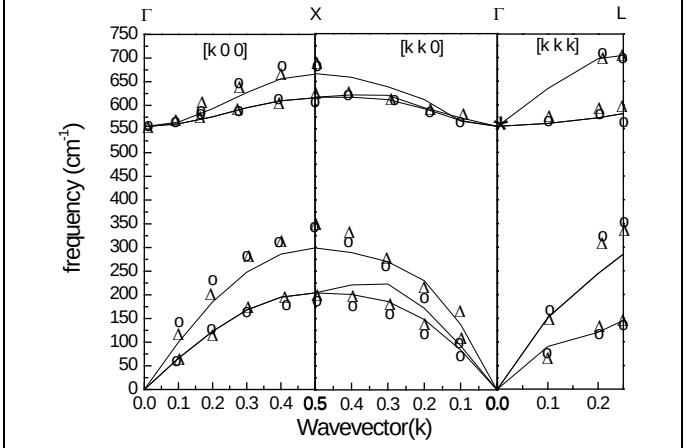


Fig. 3(a) Solid line represents the obtained phonon dispersion curve. Triangles represent the results of Dario G et.al. (1) while circle represent the results of Bechstedt F et.al.(21)

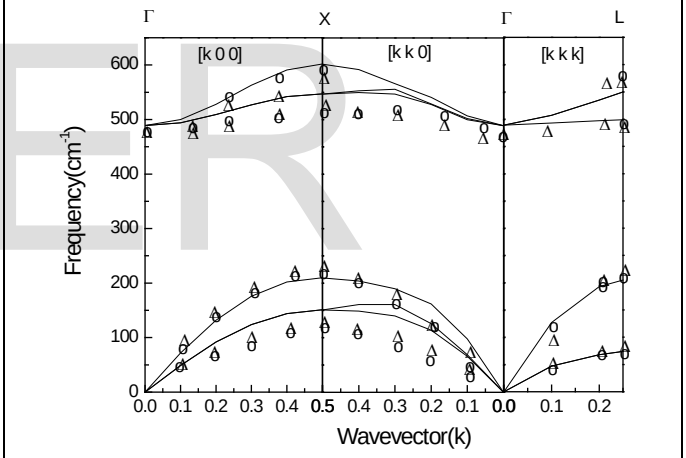


Fig. 4(a) Solid line represents the obtained phonon dispersion curve. Triangles represent the results of Dario G et.al. (1) while circle represent the results of Bechstedt F et.al.(21)

The lattice constant is minimum for BN and maximum for InN. Same observation is given by [8]. The interatomic interaction of group-III nitrides decreases in the sequences BN - AlN - GaN - InN. It is clear from the phonon dispersion curve of BN, GaN, AlN and InN that the present calculation is well in agreement with calculated results. The calculated results at zone centre and zone boundary for BN, GaN compared with results of [1, 6] and for AlN and InN compared with [21,2] are given in Table III, V ,IV and VI .

TABLE III, ZC AND ZB PHONONS OF BN

	TO (Γ)	TO1 (X)	TO2 (X)	TA (X)	LA (X)	LA (L)	TA (L)	TO1 (L)	TO2 (L)
Present calculation	1045	1049	1009	886	590	420	942	1040	1082
Ref.1	1060	1150	1015	935	700	495	950	1000	1120
Ref.6	1055	1150	1050	900	690	500	1000	1010	1150

TABLE IV, ZC AND ZB PHONONS OF ALN

	TO (Γ)	TO1 (X)	TO2 (X)	TA (X)	LA (X)	LA (L)	TA (L)	TO1 (L)	TO2 (L)
Present calculation	655	705	487	676	254	670	194	680	480
Ref. 21	665	715	590	670	340	650	220	720	580
Ref.2	660	720	580	630	310	600	200	720	600

TABLE V, ZC AND ZB PHONONS OF GAN

	TO (Γ)	TO1 (X)	TO2 (X)	TA (X)	LA (X)	LA (L)	TA (L)	TO1 (L)	TO2 (L)
Present calculation	555	204	299	616	666	285	582	705	145
Ref.1	557	200	350	625	690	340	595	700	145
Ref.6	555	190	350	610	700	360	550	700	142

TABLE VI, ZC AND ZB PHONONS OF INN

	TO (Γ)	TO1 (X)	TO2 (X)	TA (X)	LA (X)	LA (L)	TA (L)	TO1 (L)	TO2 (L)
Present calculation	489	602	547	210	151	74	205	499	560
Ref. 21	470	560	520	230	120	80	225	480	570
Ref.2	470	570	508	215	110	70	215	490	580

4. PHONON DENSITY OF STATE

The various thermodynamical properties can be calculated from the frequency distribution function g(ν) of normal modes of vibration of a solid. We have calculated the phonon density of state of AlN, BN, InN and GaN by applying sampling method. . In this method one solve for the eigen value of the dynamical matrix at the maximum possible number of points that form a mesh in the periodical section of the first BZ of the reciprocal lattice. A sorting of different frequencies, with proper weighing factor, leads to the evaluation of g(ν) In the present investigation the dynamical matrix (6X6) is solved at 48 non-equivalent points in the first BZ to generate a large number of frequencies for a large number of uniformly distributed points in the first BZ and then to approximate the spectrum by using a normalized histogram. We have calculated the frequency distribution function g(ν) with a reasonable accuracy by using 48 non- equivalent points. The frequency thus calculated on these non equivalent points with statistical weights provides the vibrational frequencies for all 1000 points of the zone, giving 6000 frequencies for a (6X6) determinant. The complete frequency range is divided into a finite number of equal intervals of width $\Delta\nu = 20$ for AlN, GaN and InN and $\Delta\nu = 30$ cm^{-1} for BN. The phonon density of states of BN, AlN,GaN and InN is given in Fig 1(b), 2(b), 3(b) and 4(b) respectively.

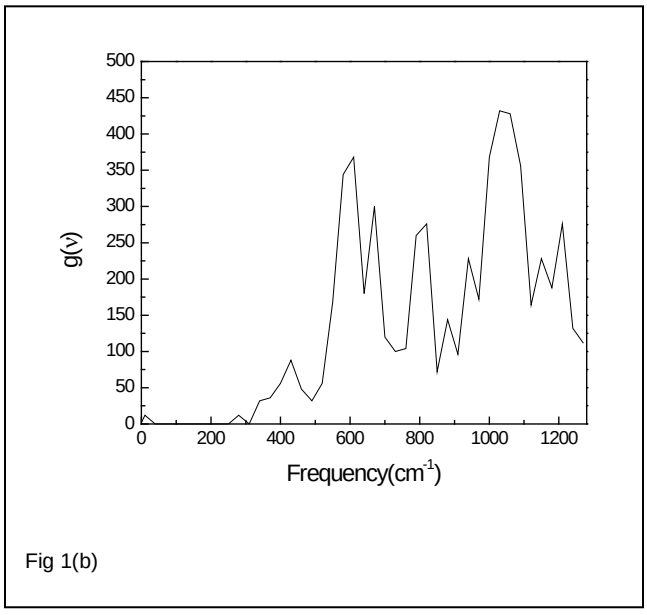


Fig 1(b)

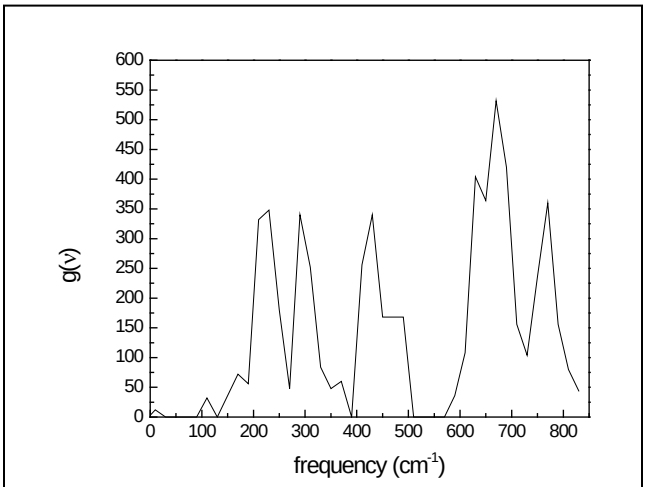


Fig 2(b)

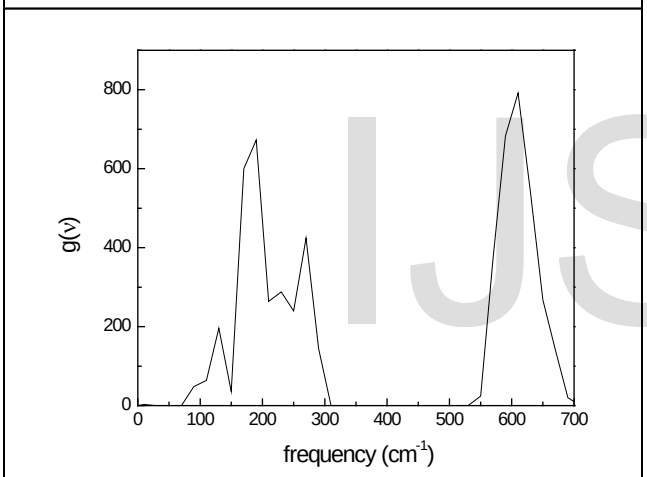


Fig 3(b)

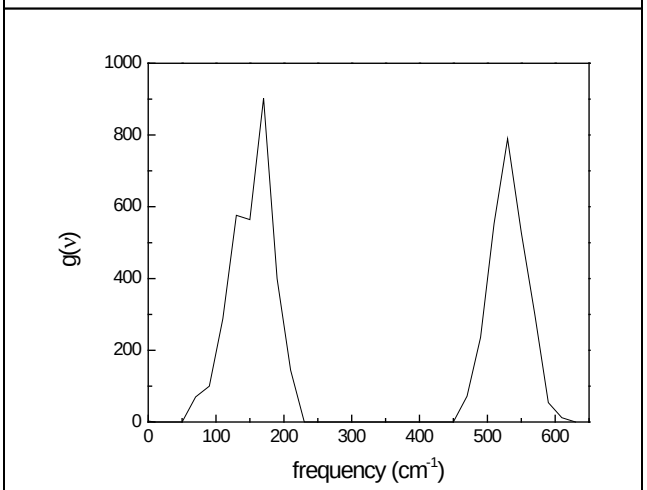


Fig 4(b)

5. CONCLUSION

In the present work we have presented a Delaunay force constant model for the calculation of lattice dynamical properties, phonon density of state (PDOS) of group-III nitrides in zinc-blende phase. The phonon dispersion curve and phonon density of state is in good agreement with existing theoretical results by using small number of parameters.

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