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Lattice Dynamical Properties of Wurtzite Phase of BN & InN

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Abstract: The group III-N semiconductors are the materials of utmost interest due to their fascinating properties and performance of devices based on these materials under extreme conditions of temperature. The large band gap of these materials makes them useful for high power, high frequency and optoelectronic devices. The important properties of the materials like Electron relaxation process, electron transport, dynamical and thermodynamical properties depend upon the excitation of phonons. So in this study we have studied the phonon and calculate the Phonon dispersion relation throughout the Brillouin zone (BZ) and phonon density of state for wurtzite phase of BN and InN. de Launey angular force (DAF) constant model has been used in this study as this model is also better choice for structures having partially covalent character. The calculated results are in excellent agreement with available experimental results at zone centre and predict phonon dispersion throughout the brillouin zone.

Keywords- Lattice dynamics, Phonons, density of states.

I. INTRODUCTION

In these days of scientific era Group-III nitride Semiconductors are considered as materials of third generation. The band gap of these materials cover a large range and also band gap can be adjusted by mixing. The band gap of InN is 1.9 eV and of BN slightly less than 5 eV [1]. It must be noted down that recently band gap of InN was found 0.7- 0.9 eV by using optical experiments but has to revise again [2]. The LED based on InN emits light in visible range and these diodes given more priority for their applications in solid state lightning [3, 4]. Due to their hardness these materials are also used for coating and can operate at high temperature and radiative environment [5]. Other important properties are large bulk modulus, high thermal conductivity, short bond length, low compressibility and high iconicity [7]. The BN and InN exists in two phases wurtzite and cubic phase, wurtzite phase is reported as much stable as compared to cubic phase.

The phonon mode study is most important for dynamical, thermo dynamical, optical transition due to phonons and structural properties It is well known that transport and thermodynamic properties are inherent for device performance [6]. Furthermore excitations of phonons also affect the non-radiative electron relaxation process and electron transport [4]. So phonon dispersion, density of state and thermodynamical are the most desired properties for these materials. So far till most experimental studies (Ist order Raman scattering and inelastic neutron scattering) investigated few phonons at zone centre and zone boundary. The theoretical studies used rigid ion model, Valence force model, ab-intio techniques and adiabatic bond charge model lack physical clarity [6, 8]. The short range de Launey angular force (DAF) model has produced the excellent lattice dynamical solution as it involves interaction of many particles through angular force. Recent studies have more focus on electronic band structure. The few available results are as Dyck et.al. [11] studied the phonon frequency of hexagonal InN at Γ -point. Bechstedt et.al. [8] calculate the phonon frequency along Γ-L direction for cubic modification of InN using ab-intio calculation. Zhang et. al [3] reports phonon dispersion curve and DOS for InN and BN using generalized gradient approximation (GGA) and local density approximation (LDA) but results obtained by both methods for InN and BN do not show agreement with each. The complete knowledge of phonons in BZ is still missing so we have decided to study the phonon of InN and BN using de Launey angular force model. Recently we have studied the cubic phase of Group-III Nitrides. In this presentation we apply DAF model to BN and InN and present (i) Phonon study throughout the Brillion Zone and (ii) Test our results with available experimental and theoretical results.

II. METHODOLOGY

In this present study to obtained phonon dispersion curve and phonon density of state of BN and InN we have used de Launey angular force constant model. This model is based on born-Von karman theory. According to it the atoms in crystal structure are assumed to be oscillating with small amplitude and exerting elastic force on each other. Amplitude of oscillation is so small that Hooke's law of elasticity is supposed to be obeyed. This model consider

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two types of interaction between atoms: Central force which acts on line joining the centers of the interacting atoms and angular force which depends upon angle made by the line joining the moving atoms and line joins their equilibrium position. This model is more suitable for the materials showing partially covalent character and it has another benefit of incorporating interaction between many particles through angular force. As this model based on short range forces so the interaction is considered upto second nearest neighbors and magnitude of the forces generally diminishes after second neighbor Interatomic interaction. The α_1 (B (In)-N) and α_2 (B (In)-B (In)) represent the force constants for central force and α'_1 (B (In)-N) and α'_2 (B (In)-B (In)) represent the force constants for angular force. The combination of both central and angular force is called non-central force and is given by

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

Where S_o and S_i are the displacements of the reference atom and ith atom. ζ represent the direction of the line joining the reference atom to the ith atom.

As wurtzite crystal structure has 4 atoms per unit cell and solving the equation 1 for each atom along three coordinate axis results in formulation of a matrix of 12x12 and solution of equation is

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

Where D (k) is (12x12) dynamical matrix and I is unit vector. By solving the dynamical matrix force constants has been obtained. The obtained force constants and experimental values of lattice constants [18, 19] are given in the table 1.

TABLE 1, INPUT PARAMETER: CALCULATED FORCE CONSTANTS AND EXPERIMENTAL VALUES OF LATTICE CONSTANTS

Element	Force constant(10^4 dyne cm^{-1})				Lattice constants (Å)	
	α_1	α'_1	α_2	α'_2	a	c
BN	19.38	5.37	6.366	-1.73	2.56	4.23
InN	11.28	1.01	1.54	0.05	3.54	5.71

By using the mass of B (In) and N and obtained force constant the frequency is calculated at zone centre, zone boundary and in the Brillion zone which is given in graph 1 and graph 2 for BN and InN respectively.

The sampling method was used to calculate the phonon density of state. In this method one solve the eigen value of the matrix at 84 point with corresponding statistical weight, which produce a mesh in irreducible section of first BZ. By sorting out different frequencies, frequency distribution function g(ν) has been evaluated.

III. RESULT

The wurtzite phase of group-III nitride semiconductors has 4 atoms in each unit cell and hence 12 degrees of freedom results in 12 frequencies in the Brillion zone. The comparison of the results of this work and other theoretical work at zone centre is given in table 2. Our result shows better agreement with the experimental results. At zone centre and at zone boundary few of the modes degenerate. In this presentation the phonon modes are studied in Brillion zone and are shown graphically in graph 1 and graph 2 respectively for BN and InN. It is observed that interatomic interactions are stronger for BN as compared to InN as the force constants are larger for BN, which is due to the smaller values of the lattice constants for BN. Also the force between B(In) and N given by α_1 is stronger as compared to the others due to minimum interatomic distance.

TABLE 2: RESULTS OF THIS WORK AND THEIR COMPARISON WITH THE AVAILABLE THEORETICAL AND EXPERIMENTAL RESULTS

Materials	Comparison with other results	E2(low)	A1(TO)	E1(TO)	E2(high)
BN	This Work	259	1006	1053	948
	Theory [3]	459	1106	1137	1041
	Experimental [6]	310	1006	1053	
InN	This Work	102	442	477	488
	Theory [3]	79	578	598	603
	Experiment [20]	87	442	477	488

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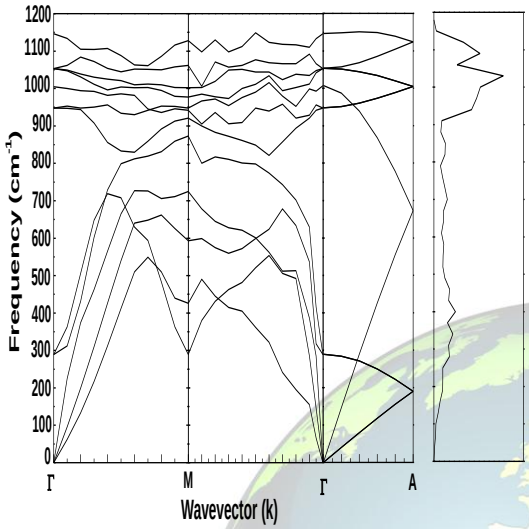
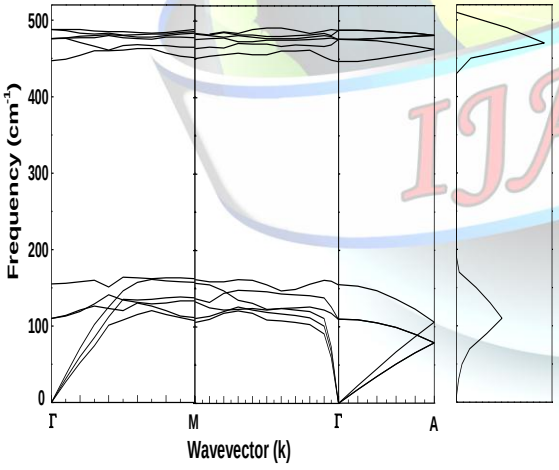


Graph 1. Phonon dispersion and phonon density of states of wurtzite BN



Graph 2. Phonon dispersion and phonon density of states of wurtzite InN

Two regions are observed in the phonon dispersion curve one corresponds to acoustical mode and second to optical mode. The optical phonon modes are much flatter as compared to the acoustical mode for both BN and InN. From the phonon dispersion curve of both it is clear that dispersion in case of BN is more than InN in both acoustical and optical modes. Even the acoustical and optical modes of BN overlaps as mass of B and N are almost same. The frequency gap can be found from zone boundary phonons with B (In) lower mass limit and nitrogen atom upper mass limit. It is found that the frequency gap between acoustical and optical modes in case of InN is more than BN, which is because of the large cation to anion mass ratio as the mass of in is more as compared to B. Moreover the maximum value of optical phonon frequency is more for BN as compared to InN due to smaller cation mass. By calculating frequency distribution function the phonon density of states has also been calculated for both BN and InN. In the phonon density of states for BN a sharp peak is observed corresponding to 1053 E1(TO) mode which is due to flatness of optical phonons in phonon dispersion curve while two small peaks one corresponding to 440 E2(low) in acoustical mode and 1006 A1(TO) in optical mode. While in InN the most sharp peak is observed corresponding to 470 E1(TO) while small peaks are also observed for 50 and 110 E1(low) corresponding to acoustical modes. The band gap between acoustical and optical modes in PDOS increases with cation to anion mass ratio. The gap observed for InN is much larger than BN. By using the density of state, the specific heat of BN and InN also has been calculated using Debye's Law in temperature range (0-400K). It is clear from the graph that specific heat increases quickly at lower temperature and then slope decreases continuously and almost becomes saturate when the specific heat approaches 3R.

The calculated results are in good agreement with existing results. According to best of our knowledge recently H Zhang et.al. [3] have studied the phonon dispersion and phonon density of states using local density approximation (LDA) and generalized gradient approximation (GGA). X. Lei et. Al.[1] have studied the phonons of BN using LDA and GGA. So it is hoped that our calculated results for Phonons in BZ, phonon DOS range will be helpful for the researchers for reference in future research.

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