International Journal of Current Research and Modern Education (IJCRME)
Impact Factor: 6.725, ISSN (Online): 2455 - 5428
(www.rdmodernresearch.com) Volume 2, Issue 2, 2017

STUDY OF PHONON PROPERTIES OF CUBIC AND WURTZITE PHASE OF InN

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Cite This Article: Daljit Singh, "Study of Phonon Properties of Cubic and Wurtzite Phase of InN", International Journal of Current Research and Modern Education, Volume 2, Issue 2, Page Number 79-83, 2017.

Abstract:

Recently many investigations were committed to the study of group-III nitride semiconductors. The group-III nitride semiconductors have many characteristics which are suitable for high-voltage, high temperature, high-reliability and high frequency devices. Group III-Nitrides have attracted a lot of attention recently, since they are promising materials for light emitting optoelectronic devices in the green and blue color spectrum. One reason is related to their extreme properties, such as high ionicity, very short bond lengths, low compressibility, high thermal conductivity and high melting temperature of the nitride subgroup of the III-V compounds is wider band gap. InN can be used for highly efficient solar cells and light emitting diodes (LEDs). In this work we are reporting the results of our theoretical investigation on the phonon properties of InN in cubic phase and wurtzite phase. The phonon properties are found by using lattice dynamical simulation method based on de Launey angular force (DAF) constant model to understand the role of phonon in these systems. The phonon dispersion curve, phonon density of states and variation of specific heat with temperature of InN in cubic phase and wurtzite phase are also drawn.

Introduction:

Group-III nitrides are considered as the capable materials for light emitting optoelectronic device throughout the visible spectrum. The wide range of band gap of the group-III semiconductors insures that breakdown electric field strength much better than that of either GaAs or Si. Moreover, it has been found that InN and GaN have inferior dielectric constants and elevated electron saturation drift velocities that can results in elevated frequency performance of devices prepared from these semiconductors (Farahmand 2001). These semiconductors are better for protective coatings due to their rigidity, elevated melting point and soaring thermal conductivity (Tutuncu et al., 2005). The free carrier concentration of group-III nitrides can also be enhanced within the channel region of a hetero junction field effect transistor (FET) ahead of that viable by modulation doping alone (Kuech et al., 1990). Due to the above stated reasons, the group III-nitride materials are of immense attention for optoelectronic device structures and power field effect transistor (FET) (Farahmand 2001). The higher refractive index of InN makes it more imperative for using it in photonic band edge design (Leroux 1999). The optoelectronic devices based on InN results in environment friendly red light emitter diodes with non toxic element replacing GaAs based devices. InN can be considered as the end member of group-III nitride semiconductors as the cation (Indium atom) is heaviest among the other atoms of the family and band gap of wurtzite InN is smallest among other members and is 1.9 eV (Harima 2002). InN can be used for highly efficient solar cells and light emitting diodes (LEDs). Mixing of InN with GaN makes it possible to have direct band gap that can emit light from infrared to ultraviolet region. The electron mobility and saturation velocity is higher, which make it ultimate material for high electron mobility devices and can operate at terahertz range. Because of such exceptional properties, it is desirable to study the phonon properties of InN. The degree of covalency and phonon properties are important design factors for the understanding of advanced applications (Loong 1998). The structural and vibrational properties are definitely the most essential ones as they decide a wide range of macroscopic behavior. In this admiration the study of lattice vibrations is of extensive attention because various thermal properties of crystals like the phonon dispersion, phonon density of states, specific heat, phase transitions and thermal expansion are related to the vibrations of atoms. Recently, the lattice dynamics of the different phases of group-III nitrides has been studied using the ab initio psuedo potential method (Tutuncu et al., 2005, Pandey et al., 2012) and an adiabatic bond charge model (Nakamura 1999). But exact information regarding dynamical properties is still missing. Therefore in this study phonon dispersion curve, phonon density of state and specific heat of InN has been calculated with the use of using de Launey angular force constant model. The InN crystallizes in two phases: cubic and wurtzite phase so phonon properties of both the phases of InN has been studied.

Methodology:

The InN crystallizes in two phases cubic and wurtzite phase. The cubic structure has couple of atoms in a unit cell with three acoustical modes and three optical modes for a wave vector while for wurtzite phase has four atoms in a unit cell with three acoustical and nine optical modes for a wave vector. The cubic phase would be sympathetic as it has higher mobility as it has lesser phonons for higher symmetry structure and is suitable for doping while wurtzite structure is considered as the most stable structure (Pereira et al., 2003) and also can

function in extreme conditions. Therefore phonon properties of both the phases of InN are strongly desired. So in this investigation the phonons in the cubic phase and wurtzite phase of InN have been calculated by using de Launey angular force constant model. As this model includes short range interaction and strength of the forces generally diminishes after second neighbor, so interatomic interaction up to second nearest neighbor is considered. Short range forces are of two types: central and angular force. The force up to second nearest neighbor are computed separately and then summed up. The different force constants are used for the central and angular forces. In this study α_1 and α_2 are the force constants for central force and α'_1 and α'_2 are force constants for angular force for first neighbor and second neighbor respectively.

A dynamical matrix of (6x6) for cubic phase has been established and is solved at zone centre and (q 0 0). The relations between force constants, frequency and elastic constants have been obtained and are given below.

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

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

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

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

Here m is the mass of In atom and M being mass of N atom, a is the lattice parameter, C_{11}, C_{12} and C_{44} are the elastic constants. By using experimental values of the elastic constants as given by (Shervin 1991; Marmalyuk 1998) and zone centre frequency (Huan 2008; Alvesa 2002) the force constants have been calculated and are given in table 1.

The dynamical matrix of (12x12) has been obtained for wurtzite phase and is solved at the zone center. The relations between some key phonon frequencies and force constants has been obtained are as given below.

$$\frac{4}{3}\left(\alpha_1 + 2\alpha_1^{'}\right) = \frac{m_1 m_2}{m_1 + m_2}\omega^2_{E_1(TO)}$$

$$\frac{4}{3}\left(\alpha_1 + 2\alpha_1^{'}\right) + 2\left(4\alpha_2 + 2\alpha_2^{'}\right) = m_2\omega^2_{A_1(TO)}$$

$$4\left(\alpha_2^2 + 25(\alpha_2^{'})^2 + 10\alpha_2\alpha_2 - \alpha_1^2\right) + \frac{16}{3}\left(\alpha_1 + 2\alpha_1^{'}\right)\left(\alpha_2 + 5\alpha_2^{'} + \alpha_1\right)$$

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

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

Here m_1 and m_2 are the mass of in atom 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.

Table 1: Calculated Force Constants

Phase	Force constant (10^4 dyne cm^{-1})			
	α_1	α_1'	α_2	α_2'
Cubic	11.28	1.01	1.54	0.05
Wurtzite	9.199	1.698	-0.1225	0.2007

Symmetry Properties:

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

$$\Gamma = 2T_2$$
$$\Gamma_{ac} = T_2\ \Gamma_{opt} = T_2$$

T_2 represent the triply degenerate modes.

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

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

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

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).

Table 2: Zone Centre Phonon Frequencies (CM^{-1}) of InN

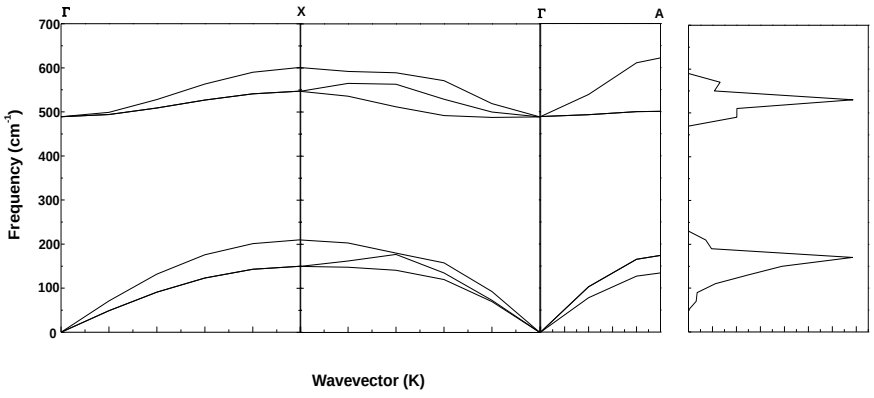
Phase	Phonon Modes	This Work	Other Theoretical results[a,b]	Other Theoretical results[c,d]	Experimental results[e,f]
Wurtzite	E_2(low)	110	79	83	87
	B_1(low)	155	239	223	
	A_1(TO)	447	570	451	447
	E_1(TO)	476	598	474	476
	E_2(high)	488	603	490	488
	B_1(high)	476	618	574	
Cubic	TO	489	470	470	489

a = Zhang et al., (2013), b= Tutuncu et al., 2002, c = Pereira et al., (2003), d = Mohammad et al., 1995, e = Tutuncu et al., (2000) f = Alvesa et al., 2002.

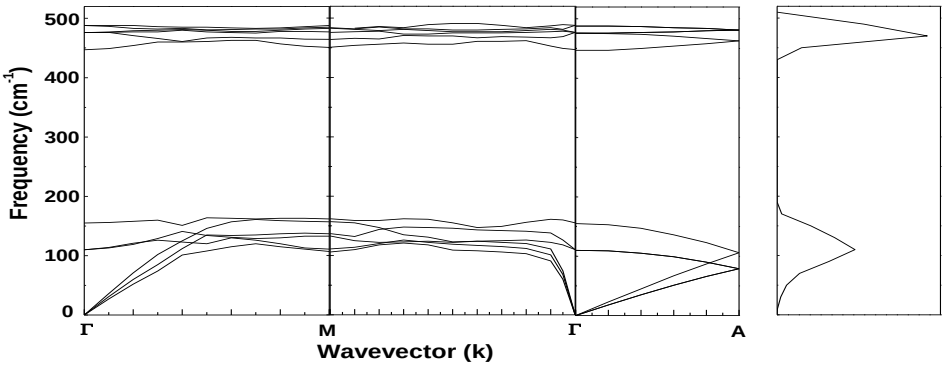
Results and Discussions:

It is clear from table II that E_1(TO), A_1(TO) and E_2 (high) mode agree with experimental results while a considerable deviation is observed in results obtained by other theoretical results with exception that E_2(low) mode show deviation. This indicate that the results of this study are in better agreement with the existing experimental results at ZC excluding E_2(low) mode. By solving the (6x6) dynamical matrix for cubic phase and (12x12) dynamical matrix for wurtzite phase along different symmetry direction and the phonon dispersion relation have been plotted and is shown in figure I and II respectively. The phonon dispersion curve has two parts. One consists of three acoustical modes having zero frequency at zone centre and second other consists of nine optical modes and few modes degenerate at the zone boundary. For wurtzite phase the doubly degenerate E_2 optical modes (77 cm^{-1} and 488 cm^{-1}) are Raman active while the A_1 (447 cm^{-1}) and doubly degenerate E_1 (476 cm^{-1}) modes are both Raman and IR active. The B_1 modes are (155 cm^{-1} and 476 cm^{-1}) are silent modes. The contribution of heavier In atom is lesser for optical phonon modes with higher frequency whiles its contribution increases for optical phonon modes with lower frequency. For B_1 (low) mode the contribution of N atom is negligible while for B_1 (high) mode the contribution of In is negligible.

It is also clear from the phonon dispersion curve that optical phonon modes show slight dispersion along different symmetry directions. The difference of mass of cation (In atom) and mass of anion (N atom) results in bigger gap between acoustical and optical branches which is be clear from the phonon dispersion curve. The frequency gap for wurtzite phase is more than cubic phase. The curve show unusual degeneracy along Γ→A direction. There are only eight modes along Γ→A direction rather than twelve modes in other directions which further reduce to four modes at A point, same trends are observed by other studies (Zhang et al., 2013, Bungaro et al., 2000). The phonon density of states for both the phases of InN shows two sharp peaks. For wurtzite phase one peak observed at 470 cm^{-1} corresponds to flattened optical modes. Whereas a small peak at 110 cm^{-1} results from combination of acoustical modes and B_1 (low) mode. For cubic phase the sharp peaks observed at 530 cm^{-1} and 170 cm^{-1} corresponds to optical and acoustical region respectively. The sharp peaks of phonon density of states results from the lesser dispersion. The variation of specific heat with temperature is also shown as graph III and graph IV. It is clear from the curve that the slope of curve decreases with increase in temperature and is attaining a constant value at higher temperature and is in agreement with $C_v = 3R$ at higher temperature.



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



Graph 2: Phonon dispersion curve and phonon density of states of wurtzite phase

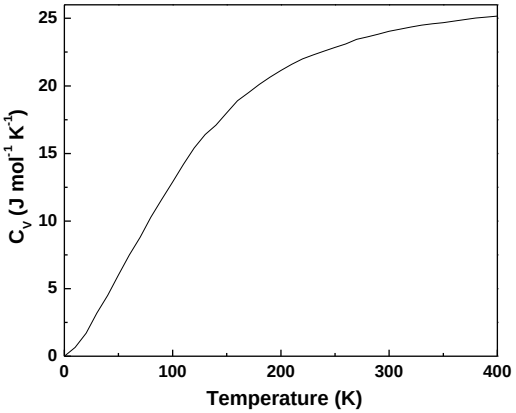


Figure 3: Variation of specific heat with temperature of cubic InN

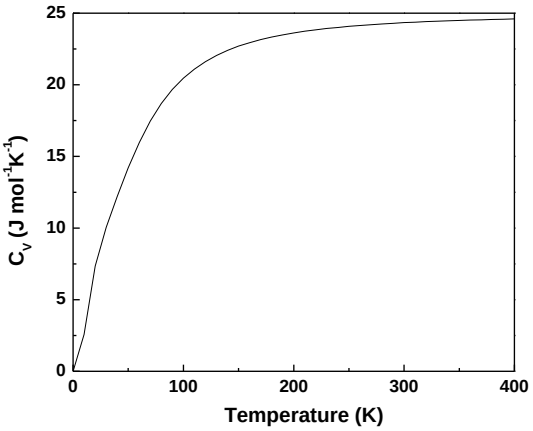


Figure 4: Variation of specific heat with temperature of wurtzite InN

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