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ZONE CENTRE PHONON MODE BEHAVIOUR OF CUBIC AND WURTZITE PHASE OF TERNARY InxGa1-xN

Ashwani Kumar* & Daljit Singh**
Department of Physics, RSD College, Ferozpur, Punjab

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Abstract:

The group-III nitrides have been acknowledged as notable materials for researchers in recent times because of their extra ordinary properties and applications. The fundamental property of these materials is their wide and direct band gap, which can also be tailored by doping. A common characteristic of these device structures is the applicability of their ternary alloys. Despite of the broad range of the ternary alloys of these group-III nitrides only some have been discussed. So in this study, zone centre phonon mode behavior of the ternary alloy $In_xGa_{1-x}N$ in both phases (cubic and wurtzite phase) has been studied and with the use of de Launey angular force constant model. The various optical phonon modes at zone centre have been calculated for both phases of $In_xGa_{1-x}N$. The content of Ga and in alloy is in the range $0<x<1$. The one mode behavior has been found for both phases of the alloy and it is found that for $In_xGa_{1-x}N$ continuous decreases in magnitude of phonon frequency with the increase in the content of In which is due to the fact that frequency varies inversely proportional to the mass, as content of In increases mass of alloy increases.

Introduction:

The group III nitrides (AlN, BN, GaN and InN) are considered as third generation semiconductors after first generation of semiconductor elements like Si and Ge and second generation semiconductor compounds InP and GaAs [1]. The possible applications of these materials are in light emitting diodes (LEDs) and laser diodes (LDs). The power of LEDs and LDs based on other semiconductors like II-VI materials decrease for emitted wavelength in blue region. Also life time for green LDs is only one hour while 100 hours for green LEDs. This prevents the commercialization of these semiconductors. On the other hand group III nitrides are the hot spots for the researchers in such applications [2]. The main interaction of these materials is due to their broad direct band gap, which can also be diverse according to the requirement. By alloying with suitable composition band gap can be varied from band gap of InN 0.7-0.9 eV to gand gap of GaN 6.3 eV (3,4), which will cover light emitting region from infra-red, visible and UV region. By using alloy of GaN doped with suitable composition of in can be used for manufacturing LEDs and electronic devices according to use [9]. GaN based semiconductor materials have large thermal conductivity, higher electron drift velocity, resistance to high voltage, useful at an elevated temperature. By changing the composition of the dopant the lattice constant and molecular weight changes, which change the refractive index, binding energy and electron mobility [5]. Higher melting point of Group-III nitrides make it useful materials for high power and high temperature microelectronic [6]. Apart from the other applications these nitrides have some other interesting properties like easy cleavage of cubic structure, conductive substrates and possibility of high doping level [7]. Due to such important application and properties these materials can meet the demands of the next generation of electronic equipment like small size, work in extreme conditions, high frequency, high efficiency and high power [1]. There are few studies of these nitrides on basis of Raman spectroscopy and by molecular beam epitaxy [8]. A. L K Teles [9] studied the The electronic, structural, and thermodynamic properties of cubic (*zinc blende*) group-III nitride ternary $In_xGa_{1-x}N$ and quaternary $Al_xIn_yGa_{(1-x-y)}N$ alloys by combining first-principles total energy calculations and cluster expansion methods. But there is clear lack of knowledge of fundamental properties such as phonon frequency and its dependence on alloy composition of these materials important for material characterization. Therefore in the present study, we have presnted the zone centre phonon mode behavior of GaN doped with In with varying composition $0<x<1$ for its both phases by using the de launey angular force constant model. The zone centre phonon frequency is studied and results found are in excellent agreement with existing experimental and theoretical results.

Methodology:

The creation of mixed crystal with special proportion of two undoped crystals results in a fresh set of crystal with physical properties which are in-between pure end members depending upon the composition of pure crystals. The properties may change in different manner with variation of composition. In some mixed crystals properties changes monotonically linearly as a function of composition while in some cases the properties may vary non-linearly (may be slightly non linearly or highly non-linear manner). In some cases, properties are different from the properties of parent crystals at all and these properties are unique to mixed crystals only.

In this study with the use of de Launey angular force constant model we have calculated the phonon frequency at zone centre of the In doped both phases of GaN with composition in range 0 to 1. In this study two parts of the interatomic interactions are taken into consideration: Central interaction (ion-ion radial interaction), which act along the straight line joining the centers of two nearest neighbors and angular force which depends upon the angle between the line joining the moving atoms makes with the line joining their mean position. As Interatomic interactions are short range, so interatomic interactions are considered for nearest and next to nearest neighbors. We shall let α_1 and α'_1 signify the force constant linked with central force and angular force of the nearest neighbor, while α_2 and α'_2 denote the force constant associated with central and angular force next nearest neighbors. In DAF model with the use of coordinates and direction cosines of the neighbors, in the equation of motion given below

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

Where S_o and S_i are the displacements of the reference atom and ith atom and
$\hat{\zeta}$ is the unit vector along the line joining the reference atom to the ith atom. By using above equation a dynamical matrix of 6x6 and 12x12 is formed for cubic phase and wurtzite phase respectively and is given by the solution of characteristic equation

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

Where D(k) is (6x6) and (12x12) dynamical matrix in case of cubic and wurtzite phase respectively and I is unit vector. The (6x6) dynamical matrix is expanded, at center of the zone to get relation between some vibrational frequencies, measured elastic constants and force constants. The relations thus obtained are as given

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

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

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

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

Here m is the mass of In_xGa_{1-x} $(xM_Y+(1-x)M_{In})$and M being mass of N. a is the lattice parameter and C_{11}, C_{12} and C_{44} are the elastic constants. By using experimental values of the zone centre frequency [13] and elastic constants as given in [14,15] the force constant has been calculated and are given in table I.

The obtained dynamical matrix of (12 x 12) is solved at zone centre results in the formulation of the relation between four unknown force constants and experimental value of frequency. The following relations between force constants and some important vibrational frequencies are obtained.

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

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

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

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

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

Here m_1 and m_2 are the mass of In_xGa_{1-x} $(xM_Y+(1-x)M_{In})$ 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 at zone centre of the binaries. Vegard's law is used to calculate the force constants for ternary alloys and mass of constituent atoms (P and Q) for any ternary alloy $P_xQ_{1-x}N$ are obtained by using Vegard's law as given below.

$$\alpha_{P_xQ_{(1-x)}N} = x\alpha_{PN} + (1-x)\alpha_{QN}$$

$$m_{P_xQ_{(1-x)}} = xm_P + (1-x)m_Q$$

Where m_P and m_Q are the masses of P (P = Al, Ga, In) and Q (Q = Al, Ga, In) and α_{PN} and α_{QN}. The calculated force constants are given in table II.

Table 1: Force constants for ternary alloy$In_xGa_{1-x}N$

Composition (x) in alloy $In_xGa_{1-x}N$	Force Constant (10^4 dyne cm^{-1})				
	α_1	α_1'	α_2	α_2'	Mass
0.0	14.06	0.98	1.95	0.15	116.39
0.2	13.49	0.99	1.87	0.13	131.462
0.4	12.92	1.01	1.74	0.09	146.534
0.6	12.35	1.01	1.71	0.08	161.606
0.8	11.78	1.02	1.63	0.06	176.678
1	11.22	1.04	1.55	0.04	191.75

Table 2: Force constants for wurtzite ternary alloy $In_xGa_{1-x}N$

Alloy	Composition (x)	Force Constant (10^4 dyne cm^{-1})				Mass In_xGa_{1-x} (10^{-24}gm)
		α_1	α_1'	α_2	α_2'	
$In_xGa_{1-x}N$	0.0	10.5253	2.8951	0.0933	0.2703	116.39
	0.2	1026008	2.65586	0.05014	0.25638	131.462
	0.4	9.994716	2.41662	0.0698	0.24462	146.534
	0.6	9.729424	2.17738	0.03618	0.22854	161.606
	0.8	9.464132	1.93814	-0.0793	0.21462	176.678
	1	9.1992	1.6989	-.1225	0.2007	191.75

Results and Discussions:

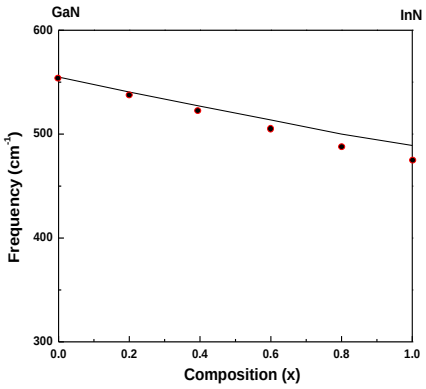

Figure 1: Phonon mode behavior of ternary $Al_xGa_{1-x}N$

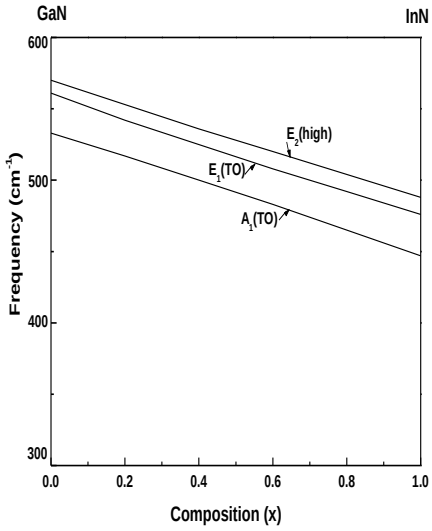

Figure 2: One mode behavior of wurtzite ternary alloy $In_xGa_{1-x}N$

It is clear from table I and II that as the dopant concentration increases the mass of mixture In_xGa_{1-x} increases and force constants decreases. The larger magnitude of force constants indicates the stronger inter atomic interaction and vice versa. It is clear from figure I for cubic phase that as the concentration of dopant (In) increases mass increases hence force constants decreases results in lowering the zone centre frequency. From figure II $In_xGa_{1-x}N$ as the concentration of dopant (In) increases the magnitude of the zone centre optical phonon frequencies (A_1(TO), E_1(TO) and E_2(high)) decreases which is in harmony with the fact that the stronger interaction results in greater value of the optical phonon frequency and vice versa. It is observed for both phases of ternary alloys that the optical phonon frequencies show linear variation with the concentration of dopant from one end member to other. This shows that this alloys exhibit one mode behavior right through the whole range of concentration.

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